797ML Handbook

Steve Linberg

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Contents

1	$\mathbf{A}\mathbf{b}$	out	9		
	1.1	Authoring guidelines	9		
	1.2	Contact	10		
	1.3	Resources	10		
2	Simple Linear Regression 11				
	2.1	TL;DR	11		
	2.2	What it does	11		
	2.3	When to do it	12		
	2.4	How to do it	12		
	2.5	How to assess it	14		
	2.6	Where to learn more	14		
	2.7	Notes	14		
3	Multiple Linear Regression 17				
	3.1	TL;DR	17		
	3.2	What it does	17		
	3.3	When to do it	17		
	3.4	How to do it	18		
	3.5	How to assess it	19		
	3.6	Where to learn more	19		
4	Logistic Regression 21				
	4.1	TL;DR	21		
	4.2	What it does	21		
	4.3	When to do it	21		
	4.4	How to do it	21		
	4.5	How to assess it	23		
	4.6	Where to learn more	25		
	4.7	Notes	25		
5	Lin	ear Discriminant Analysis (LDA)	27		
		TL:DB	27		

	5.2	What it does	27		
	5.3	When to do it	28		
	5.4	How to do it	28		
	5.5	How to assess it	28		
	5.6	Where to learn more	30		
6	TODO: Quadratic Discriminant Analysis				
	6.1	TL;DR	31		
	6.2	What it does	31		
	6.3	When to do it	31		
	6.4	How to do it	31		
	6.5	How to assess it	31		
	6.6	Where to learn more	32		
7		DO: Naive Bayes	33		
	7.1	TL;DR	33		
	7.2	What it does	33		
	7.3	When to do it	33		
	$7.4 \\ 7.5$	How to do it	33 33		
	7.6	Where to learn more	33		
	7.0	where to learn more	აა		
8		DO: K-Nearest Neighbors	35		
	8.1	TL;DR	35		
	8.2	What it does	35		
	8.3 8.4	When to do it	35 35		
	8.5	How to assess it	35		
	8.6	Where to learn more	36		
	0.0	Where to learn more	50		
9		DO: Poisson Regression	37		
	9.1 9.2	TL;DR	37 37		
	9.2	What it does	37		
	9.4	How to do it	$\frac{37}{37}$		
	9.5	How to assess it	37		
	9.6	Where to learn more	37		
10	тОІ	DO: Cross-Validation	39		
10		TL;DR	39		
		What it does	39		
		When to do it	39		
		How to do it	39		
		How to assess it	39		
	10.6	Where to learn more \dots	39		
11	TOI	DO: Bootstrap	41		

CONTENTS	5
----------	---

	11.1	TL;DR	41
		What it does	41
		When to do it	41
		How to do it	41
	11.5	How to assess it	41
		Where to learn more	41
12	TOI	OO: Best Subset Selection	43
		TL;DR	43
		What it does	43
		When to do it	43
		How to do it	43
		How to assess it	43
		Where to learn more	44
12	тот	OO: Stepwise Selection	45
10		TL;DR	45
		What it does	45
		When to do it	45
		How to do it	45
		How to assess it	45
		Where to learn more	45
	10.0	Whole to load more and a second more and a secon	10
14	TOI	OO: Ridge Regression	47
	14.1	$TL; DR \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	47
	14.2	What it does	47
	14.3	When to do it	47
	14.4	How to do it \ldots	47
		How to assess it	47
	14.6	Where to learn more	47
15	TOI	OO: Lasso	49
		TL;DR	49
		What it does	49
		When to do it	49
		How to do it	49
		How to assess it	49
		Where to learn more \dots	49
16	тог	OO: Principal Component Regression	51
10		TL;DR	51
		What it does	51
		When to do it	51
		How to do it	51
		How to assess it	51
		Where to learn more	52
	±0.0	**************************************	02

6 CONTENTS

	53
17.1 TL;DR	. 53
17.2 What it does	
17.3 When to do it	
17.4 How to do it	
17.5 How to assess it	
17.6 Where to learn more	
18 TODO: Random Forests	55
18.1 TL;DR	
18.2 What it does	
18.3 When to do it	
18.4 How to do it	
18.5 How to assess it	
18.6 Where to learn more	
10.0 Where to retain more	. 00
19 TODO: Boosting	57
19.1 TL;DR	
19.2 What it does	
19.3 When to do it	
19.4 How to do it	
19.5 How to assess it	
19.6 Where to learn more	. 57
20 TODO: Bayesian Additive Regression Trees	59
20.1 TL;DR	
	- 59
20.2 What it does	. 59
20.2 What it does	. 59 . 59
20.2 What it does	. 59 . 59 . 59
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it	. 59 . 59 . 59 . 59
20.2 What it does	. 59 . 59 . 59 . 59
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines	. 59 . 59 . 59 . 59 . 60
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR	. 59 . 59 . 59 . 60 61 . 61
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines	. 59 . 59 . 59 . 60 61 . 61
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR	. 59 . 59 . 59 . 60 61 . 61
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does	. 59 . 59 . 59 . 60 61 . 61 . 61
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it	. 59 . 59 . 59 . 60 61 . 61 . 61
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it 21.4 How to do it	. 59 . 59 . 59 . 60 61 . 61 . 61
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it 21.4 How to do it 21.5 How to assess it 21.6 Where to learn more	. 59 . 59 . 59 . 60 61 . 61 . 61 . 61
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it 21.4 How to do it 21.5 How to assess it 21.6 Where to learn more 22 TODO: Principal Component Analysis	. 59 . 59 . 59 . 60 61 . 61 . 61 . 62
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it 21.4 How to do it 21.5 How to assess it 21.6 Where to learn more 22 TODO: Principal Component Analysis 22.1 TL;DR	. 59 . 59 . 59 . 60 61 . 61 . 61 . 62 63
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it 21.4 How to do it 21.5 How to assess it 21.6 Where to learn more 22 TODO: Principal Component Analysis 22.1 TL;DR 22.2 What it does	. 59 . 59 . 59 . 60 61 . 61 . 61 . 62 63 . 63
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it 21.4 How to do it 21.5 How to assess it 21.6 Where to learn more 22 TODO: Principal Component Analysis 22.1 TL;DR 22.2 What it does 22.3 When to do it	. 59 . 59 . 59 . 60 61 . 61 . 61 . 62 63 . 63 . 63
20.2 What it does 20.3 When to do it 20.4 How to do it 20.5 How to assess it 20.6 Where to learn more 21 TODO: Support Vector Machines 21.1 TL;DR 21.2 What it does 21.3 When to do it 21.4 How to do it 21.5 How to assess it 21.6 Where to learn more 22 TODO: Principal Component Analysis 22.1 TL;DR 22.2 What it does	. 59 . 59 . 59 . 60 61 . 61 . 61 . 62 63 . 63 . 63

CONTENTS		7

	22.6	Where to learn more	64
23	TO	DO: K-Means Clustering	65
	23.1	TL;DR	65
	23.2	What it does	65
	23.3	When to do it	65
	23.4	How to do it	65
	23.5	How to assess it	65
	23.6	Where to learn more	66
24	TO	DO: Hierarchical Clustering	67
	24.1	TL;DR	67
	24.2	What it does	67
	24.3	When to do it	67
	24.4	How to do it	67
	24.5	How to assess it	67
	24.6	Where to learn more	68

8 CONTENTS

About

This book is being written as part of a final project for 797ML at UMass Amherst, spring 2022. It contains a simple reference and breakdown for a couple of dozen core methods used in machine learning.

The intent is twofold:

- 1. Serve as a reference for the basics of the material covered in the class, using language and examples that are as simple as possible to explain the core concepts and how to do them;
- 2. Force myself to learn these techniques better by carrying out the above.

The main purpose of this work is to be *simple*, not to be *comprehensive*. We won't cover every facet of every technique, or every possible permutations of outcomes. The goal is to simply express the broad strokes and core concepts in a way that can be easily remembered, and to serve as a jumping-off point when more information is needed.

1.1 Authoring guidelines

The goal is to have no more than a few short paragraphs for each section, and to keep each explanation of the meanings of outcome variables to one sentence each.

Each chapter will have a TL;DR section at the top with *one-sentence answers* to following questions:

- What it does (answer the question starting with "It...")
- When to do it
- · How to do it
- · How to assess it

and it will be possible to skim through the book, just surfing the TL;DR at the top of each chapter, and get a reasonable overview without reading the rest. The rest of each chapter will deliver more fleshed-out, but *short*, answers to the same questions, covering the basics and the most general concepts.

1.2 Contact

Steve Linberg: steve@slinberg.net || https://slinberg.net

Project home: https://stevelinberg.github.io/797MS-handbook/ Github repo: https://github.com/stevelinberg/797MS-handbook

1.3 Resources

A lot of the material from this work is from the class textbook, James et al. [2021]. I also find UNC geneticist Josh Starmer's StatQuest video series on YouTube to be immensely helpful for simple explanations of statistics and machine learning concepts. His website statquest.org has many additional useful resources.

Simple Linear Regression

2.1 TL;DR

What it does Looks to see how well a single predictor variable predicts an outcome, like how well do years of education predict salary?

When to do it When you want to see if pretty much the simplest possible model provides enough of an explanation of variance for your purposes

How to do it With the lm() function, among other ways

How to assess it Look for a significant p-value for the predictor, and a reasonable \mathbb{R}^2

Note "Linear" does not necessarily mean "straight" in this context; a linear regression line can curve.

2.2 What it does

Simple linear regression is where it all begins; among the simplest of all of the regression techniques in analysis, which attempts to estimate a slope and an intercept line for a set of observations using a single predictor variable X and an output variable Y. It uses ordinary least squares (OLS) to build its model, looking for the line through the mean of X and Y that has the smallest sum of squares between the predicted and observed values.

The figure above shows a plot of a simple linear regression, attempting to use the variable TV to predict Sales. The blue line is the line defined by the regression with its Y intercept and slope; the red dots are the actual observations of Sales for each measure of the predictor TV on the X axis. The thin blue lines are the error in the prediction.

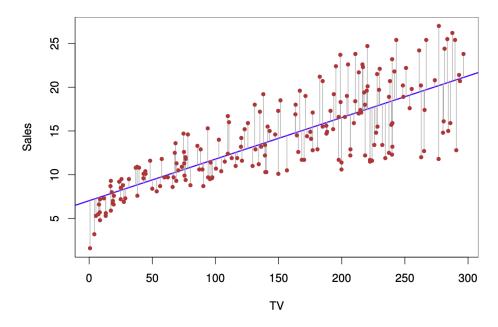


Figure 2.1: Simple linear regression plot (source: James et al. [2021], p. 62)

2.3 When to do it

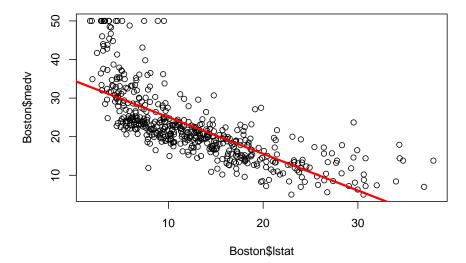
It is a simple first step for looking at data to see if there is an easy single-variable model that does a reasonable job predicting outcomes using one predictor variable. Sometimes, it can be good enough! It has the advantage of being easy to execute, to understand and to communicate, and the value of these factors should not be underestimated. Communicating with non-specialists is an important aspect of a data scientist's job.

Linear regression requires a dataset with a continuous outcome variable; it is easiest and most effective if the predictor variable is also numeric, whether continuous or discrete. It is possible to do linear regression with non-numeric predictors, such as true/false or ordered responses, by converting the predictors to a numeric scale.

2.4 How to do it

This example from James et al. [2021] shows a simple linear regression of **medv** onto **lstat**, attempting to predict median housing prices from percentage of "lower-status" population in the Boston data set from the late 1970s.

```
lm.fit <- lm(medv ~ lstat, data = Boston)
plot(Boston$lstat, Boston$medv)
abline(lm.fit, lwd = 3, col = "red")</pre>
```



The results of the regression are stored in the output of lm(), and may be viewed with summary():

summary(lm.fit)

```
##
## Call:
## lm(formula = medv ~ lstat, data = Boston)
## Residuals:
##
      Min
               1Q Median
                               3Q
                                      Max
## -15.168 -3.990 -1.318
                            2.034
                                   24.500
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 34.55384
                          0.56263
                                    61.41
                                            <2e-16 ***
                          0.03873 -24.53
## lstat
              -0.95005
                                            <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 6.216 on 504 degrees of freedom
## Multiple R-squared: 0.5441, Adjusted R-squared: 0.5432
## F-statistic: 601.6 on 1 and 504 DF, p-value: < 2.2e-16
```

2.5 How to assess it

The output contains a lot of information, but the key points are:

- Adjusted R-squared: 0.5432 is the percentage of the variation in the model that is explained by the fit's prediction, compared to just looking at how much the observations vary from their own average with no predictor variable.
- Residual standard error: 6.216 is "the average amount that the response will deviate from the true regression line", or the standard deviation of the error. In this case, since the unit of medv is in thousands of dollars, it means the average prediction will be off by \$6,216.
- p-value: < 2.2e-16 (basically zero) means that the model is (very) statistically significant, with a near-zero percent chance that the data in this set could have resulted from a random draw from the (unknown) population if there were no relationship between medv and lstat.
- Estimated intercept of 34.55 is the Y intercept on the graph, or the estimated value of medv when lstat is zero.
- Estimated (1stat): -0.95 is the estimated coefficient of 1stat, or the amount that medv changes by for each unit change in 1stat.

The intercept and coefficient are β_0 and β_1 , respectively, of the linear regression formula

$$\hat{y} = \hat{\beta_0} + \hat{\beta_1} x$$

Substituting the coefficients and variables, we transform this to:

$$\widehat{\text{medv}} = 34.55 - 0.95 \times \text{lstat}$$

The low p-value shows that there is (almost) definitely a relationship between medv and lstat, but the R^2 of 0.54 shows that the model only explains slightly more than half of the variation in the data. It's not a bad start, but we would probably want to find a model that explains more of it.

2.6 Where to learn more

- Chapter 3 3.1 in James et al. [2021]
- StatQuest: Linear Regression this goes into good depth on the meaning of the F statistic as well, and how it used to calculate the p value.

2.7 Notes

You can also do a scatterplot in ggplot2 and add a regression line with geom_smooth(); it doesn't show the coefficients or other output information, but it gives a quick visual that's a little prettier than the base R plot:

2.7. NOTES 15

```
ggplot(data = Boston, aes(x = lstat, y = medv)) +
    geom_point(alpha = 0.5) +
    geom_smooth(method = "lm", formula = y ~ x) +
    geom_hline(yintercept = mean(Boston$medv), linetype = "dashed", color = "red") +
    geom_vline(xintercept = mean(Boston$lstat), linetype = "dashed", color = "darkgreen") +
    theme_minimal()
```

The means of lstat and medv are shown with dashed red and green lines, showing that the regression line goes through the center of the data.

Multiple Linear Regression

3.1 TL;DR

What it does Looks to see how well multiple predictor variables predict an outcome, like how well do years of education and age predict salary?

When to do it When a simple linear regression doesn't provide a good enough explanation of variance, and you want to see if adding additional variables provides a better one

How to do it With the lm() function, utilizing more than one predictor How to assess it Look for significant p-values for the predictors, and a reasonable adjusted- R^2

3.2 What it does

Multiple linear regression is the first natural extension of simple linear regression. It allows for more than one predictor variable to be specified. It is also possible to combine predictors in interactions, to find out if combinations of predictors have different effects than simply adding them to the model. XXX explain/demo

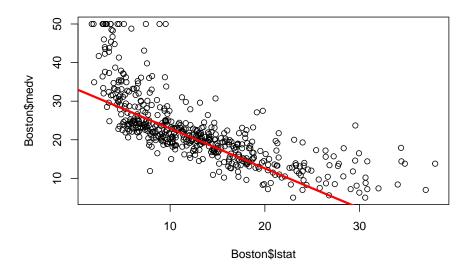
3.3 When to do it

Use multiple linear regression when a simple linear regression doesn't provide a good enough explanation of the variance you're observing, and you want to see if adding more predictors provides a better fit. Typically, this would be in response to either a low \mathbb{R}^2 that leaves a lot of unexplained variance, or even just a visual conclusion drawn from seeing a plot of a linear model with an unsatisfactory regression line.

3.4 How to do it

Use the same lm() function, with more than one predictor in the formula.

```
lm.fit <- lm(medv ~ lstat + age, data = Boston)
plot(Boston$lstat, Boston$medv)
abline(lm.fit, lwd = 3, col = "red")</pre>
```



As with simplr linear regression, the results of the regression are stored in the output of lm(), and may be viewed with summary():

```
summary(lm.fit)
```

```
##
## lm(formula = medv ~ lstat + age, data = Boston)
##
## Residuals:
      Min
                1Q
                   Median
                                3Q
                                       Max
## -15.981 -3.978
                   -1.283
                             1.968
                                    23.158
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 33.22276
                           0.73085 45.458 < 2e-16 ***
## lstat
               -1.03207
                           0.04819 -21.416 < 2e-16 ***
                0.03454
                           0.01223
                                     2.826 0.00491 **
## age
## ---
```

```
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 6.173 on 503 degrees of freedom
## Multiple R-squared: 0.5513, Adjusted R-squared: 0.5495
## F-statistic: 309 on 2 and 503 DF, p-value: < 2.2e-16</pre>
```

All of the same parameters are there, with the addition of one coefficient line for each parameter specified in the model. Each coefficient has its own estimate, standard error, t value and p value, and should be evaluated independently.

The main task is to get the ideal subset of parameters that provide the best fit, which can involve a lot of trial and error. Forward selection involves starting with a null model (no parameters) and trying all available parameters to see which has the lowest p-value, and adding that and continuing until the parameters are no longer significant or don't reduce the adjusted R^2 ; Backward selection starts with all parameters and removes the least significant one at a time until all remaining parameters are significant; Mixed selection starts with forward selection but also removes parameters that lose their significance along the way.

Other tidbits:

- interaction terms can be specified with syntax like lstat * age, which adds lstat, age and lstat * age as predictors; if an interaction is significant but an individual predictor from the interaction isn't, it should still be left in the model
- nonlinear transformations like age² can be added by escaping them inside the I() function, like I(age²), to escape the ^ character inside the formula

3.5 How to assess it

With the exception of the additional information for each parameter, the assessment is the same as for simple linear regression.

In the example above, we see that the addition of age only added a tiny bit of improvement to the model from the simple linear regression on just lstat. Other variables, or combinations of variables, might do a better job.

3.6 Where to learn more

• Chapter 3.2 in James et al. [2021]

Logistic Regression

4.1 TL;DR

What it does Models the *probability* that an observation falls into one of two categories

When to do it When you are trying to predict a categorical variable with two possible outcomes, like true/false, instead of something continuous like in linear regression

How to do it With the glm() function, specifying family = "binomial"

How to assess it Look for a significant p-value for the predictor, and assess its accuracy against training data

4.2 What it does

Logistic regression is used to make a prediction about whether an observation falls into one of two categories. This is an alternative to linear regression, which predicts a continuous outcome. A logistic regression results in a model that gives the probability of Y given X.

4.3 When to do it

As the TL;DR says: When you are trying to predict a categorical variable with two possible outcomes, like true/false, instead of something continuous.

4.4 How to do it

First, it's important to note that logistic regression will give better results when the model is fit using *held out* or *training* data, and then tested against other

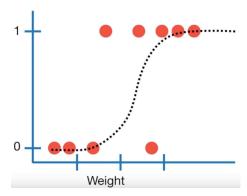


Figure 4.1: Linear regression plot (source: StatQuest)

data, to help avoid overfitting. It is not required, but it's recommended where possible.

First, before that, fit a model using glm(), making sure in this case that we have a categorical value to test for:

```
data(Boston)
boston <- Boston %>%
 mutate(
    # Create the categorical crim_above_med response variable
    crim_above_med = as.factor(ifelse(crim > median(crim), "Yes", "No")),
    # Also make a numeric version of crim_above_med for the plot
    crim_above_med_num = ifelse(crim > median(crim), 1, 0)
  )
boston.fits <- glm(crim_above_med ~ nox, data = boston, family = binomial)
summary(boston.fits)
##
## Call:
## glm(formula = crim_above_med ~ nox, family = binomial, data = boston)
##
## Deviance Residuals:
##
        Min
                   1Q
                         Median
                                        3Q
                                                Max
## -2.27324 -0.37245 -0.06847
                                  0.39620
                                             2.53124
##
## Coefficients:
##
               Estimate Std. Error z value Pr(>|z|)
## (Intercept) -15.818
                             1.386 -11.41
                                              <2e-16 ***
## nox
                 29.365
                             2.599
                                     11.30
                                              <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

```
## (Dispersion parameter for binomial family taken to be 1)
##
## Null deviance: 701.46 on 505 degrees of freedom
## Residual deviance: 320.39 on 504 degrees of freedom
## AIC: 324.39
##
## Number of Fisher Scoring iterations: 6
```

We can see the that p value for the nox variable is nearly 0, suggesting a strong association between nox and crim_above_med.

Now split the data into training and test sets, using, say, 80% of the data for training:

```
set.seed(1235)
boston.training <- rep(FALSE, nrow(boston))
boston.training[sample(nrow(boston), nrow(boston) * 0.8)] <- TRUE
boston.test <- !boston.training</pre>
```

Fit the above model to the training data:

```
boston.fits <-
glm(
    crim_above_med ~ nox,
    data = boston,
    subset = boston.training,
    family = binomial
)</pre>
```

And use the fit to predict the test data with predict():

```
boston.probs <- predict(boston.fits, boston[boston.test,], type = "response")</pre>
```

4.5 How to assess it

Yes 5 49

##

Assess the accuracy of the predictions by building a confusion matrix, using the same values ("No" and "Yes" in this case) as contained in the outcome variable we want to predict:

```
boston.pred <- rep("No", sum(boston.test))
boston.pred[boston.probs > 0.5] <- "Yes"
table(boston.pred, boston[boston.test,]$crim_above_med)

##
## boston.pred No Yes
##
No 36 12</pre>
```

The above table shows that the model correctly predicted crim_above_med from

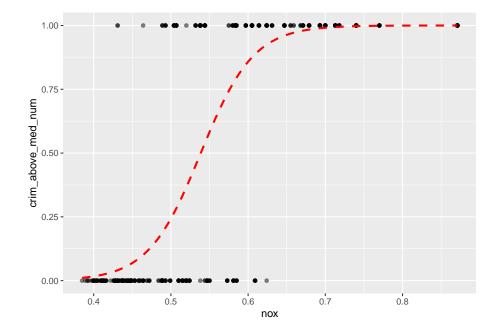
nox 85 times out of 102, with 5 false positives and 12 false negatives. The accuracy of the model can be computed via the mean() of how often the predictions match the test data, a neat trick:

```
mean(boston.pred == boston[boston.test,]$crim_above_med)
```

[1] 0.8333333

The regression can be plotted with ggplot2 and the stat_smooth() function, utilizing the glm method, like so:

```
ggplot(boston, aes(x = nox, y = crim_above_med_num)) +
geom_point(alpha = .5) +
stat_smooth(
  method = "glm",
  formula = y ~ x,
  se = FALSE,
  method.args = list(family = binomial),
  col = "red",
  lty = 2
)
```



This shows that an observation with a nox value of 0.6 would have around a 90% probability of crim_above_med being true, or 1, while an observation with a nox value of 0.5 would only have around a 25% probability of crim_above_med being true.

4.6 Where to learn more

• Chapter 4 - 4.4 in James et al. [2021]

• StatQuest: Logistic Regression

4.7 Notes

Like with linear regression, the "multiple" flavor of logistic regression works much the same way, with the specification of additional predictors in the formula, and so doesn't really warrant a whole chapter of its own. The selection of variables requires some effort, and is addressed under best subser selection.

Linear Discriminant Analysis (LDA)

5.1 TL;DR

What it does Separates observations into categories, like logistic regression, but using category means and variances for separation rather than probabilities

When to do it When exploring various classifiers to see which works best for a given data set

How to do it With the lda() function, using training and testing setsHow to assess it Assess the accuracy of the predictions on the test set after training

5.2 What it does

Similar to principal component analysys (PCA), LDA reduces dimensionality and finds the best single axis to separate two (or more) groups of observations into categories using a least-squares method of distance from a mean. Like PCA, it returns a set of new axes for the data, organized by importance, so that the first axis is the one that explains the largest amount of variance, and so on, down to p-1 axes where p is the number of categories/dimensions.

So, LDA will return 3 axes for a set of observations with 4 categories, or 1 for a set of observations with 2 categories. Each axis will have a loading score that indicates which variables had the biggest impacts on it.

5.3 When to do it

When you want to see if it will work better than other classification methods! It should always be tried along with other classifiers like logistic regression, quadratic discriminant analysis, and Naive Bayes.

5.4 How to do it

Again, using the Boston data from the logistic regression chapter:

```
data(Boston)
boston <- Boston %>%
  mutate(
    # Create the categorical crim_above_med response variable
    crim_above_med = as.factor(ifelse(crim > median(crim), "Yes", "No")),
  )
```

We again split the data into training and test sets:

```
set.seed(1235)
boston.training <- rep(FALSE, nrow(boston))
boston.training[sample(nrow(boston), nrow(boston) * 0.8)] <- TRUE
boston.test <- !boston.training</pre>
```

And fit the above model to the training data using the lda() function from the MASS library¹ (note: there is no family argument as with glm(), but the calls are otherwise identical):

```
boston_lda.fits <-
  lda(
    crim_above_med ~ nox,
    data = boston,
    subset = boston.training,
)</pre>
```

5.5 How to assess it

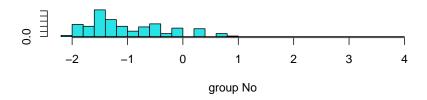
The fit can be directly examined:

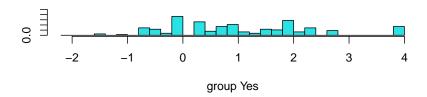
```
boston_lda.fits

## Call:
## lda(crim_above_med ~ nox, data = boston, , subset = boston.training)
##
```

¹Note to my fellow New Englanders: the MASS library is named for a book titled "Modern Applied Statistics with S", and although it does contain an earlier version of the Boston dataset (among many others), it has nothing to do with Massachusetts, and our Boston dataset comes from the ISLR2 library.

```
## Prior probabilities of groups:
##
          No
                   Yes
## 0.5247525 0.4752475
##
## Group means:
##
             nox
## No 0.4710519
## Yes 0.6357865
##
## Coefficients of linear discriminants:
##
            LD1
## nox 12.29052
And plotted:
plot(boston_lda.fits)
```





The fit should be used to predict the test data, and the model can be assessed on its results:

boston_lda.pred <- predict(boston_lda.fits, boston[boston.test,])
table(boston_lda.pred\$class, boston[boston.test,]\$crim_above_med)</pre>

In this example, LDA made the correct categorization 87 times out of 102, with 3 false positives and 12 false negatives. Again, we can compute the prediction accuracy by the mean of the correct-to-wrong guesses:

mean(boston_lda.pred\$class == boston[boston.test,]\$crim_above_med)

[1] 0.8529412

5.6 Where to learn more

- Chapter 4.4.1 4.4.2 in James et al. [2021]
- StatQuest: Linear Discriminant Analysis

TODO: Quadratic Discriminant Analysis

6.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

6.2 What it does

TODO

6.3 When to do it

TODO

6.4 How to do it

TODO

6.5 How to assess it

6.6 Where to learn more

TODO: Naive Bayes

7.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

7.2 What it does

TODO

7.3 When to do it

TODO

7.4 How to do it

TODO

7.5 How to assess it

TODO

7.6 Where to learn more

TODO: K-Nearest Neighbors

8.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

8.2 What it does

TODO

8.3 When to do it

TODO

8.4 How to do it

TODO

8.5 How to assess it

8.6 Where to learn more

TODO: Poisson Regression

9.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

9.2 What it does

TODO

9.3 When to do it

TODO

9.4 How to do it

TODO

9.5 How to assess it

TODO

9.6 Where to learn more

TODO: Cross-Validation

10.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

10.2 What it does

TODO

10.3 When to do it

TODO

10.4 How to do it

TODO

10.5 How to assess it

TODO

10.6 Where to learn more

TODO: Bootstrap

11.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

11.2 What it does

TODO

11.3 When to do it

TODO

11.4 How to do it

TODO

11.5 How to assess it

TODO

11.6 Where to learn more

TODO: Best Subset Selection

12.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

12.2 What it does

TODO

12.3 When to do it

TODO

12.4 How to do it

TODO

12.5 How to assess it

TODO: Stepwise Selection

13.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

13.2 What it does

TODO

13.3 When to do it

TODO

13.4 How to do it

TODO

13.5 How to assess it

TODO

13.6 Where to learn more

TODO: Ridge Regression

14.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

14.2 What it does

TODO

14.3 When to do it

TODO

14.4 How to do it

TODO

14.5 How to assess it

TODO

14.6 Where to learn more

TODO: Lasso

15.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

15.2 What it does

TODO

15.3 When to do it

TODO

15.4 How to do it

TODO

15.5 How to assess it

TODO

15.6 Where to learn more

TODO: Principal Component Regression

16.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

16.2 What it does

TODO

16.3 When to do it

TODO

16.4 How to do it

TODO

16.5 How to assess it

TODO: Bagging

17.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

17.2 What it does

TODO

17.3 When to do it

TODO

17.4 How to do it

TODO

17.5 How to assess it

TODO

17.6 Where to learn more

TODO: Random Forests

18.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

18.2 What it does

TODO

18.3 When to do it

TODO

18.4 How to do it

TODO

18.5 How to assess it

TODO

18.6 Where to learn more

TODO: Boosting

19.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

19.2 What it does

TODO

19.3 When to do it

TODO

19.4 How to do it

TODO

19.5 How to assess it

TODO

19.6 Where to learn more

TODO: Bayesian Additive Regression Trees

20.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

20.2 What it does

TODO

20.3 When to do it

TODO

20.4 How to do it

TODO

20.5 How to assess it

TODO: Support Vector Machines

21.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

21.2 What it does

TODO

21.3 When to do it

TODO

21.4 How to do it

TODO

21.5 How to assess it

TODO: Principal Component Analysis

22.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

22.2 What it does

TODO

22.3 When to do it

TODO

22.4 How to do it

TODO

22.5 How to assess it

TODO: K-Means Clustering

23.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

23.2 What it does

TODO

23.3 When to do it

TODO

23.4 How to do it

TODO

23.5 How to assess it

TODO: Hierarchical Clustering

24.1 TL;DR

What it does TODO When to do it TODO How to do it TODO How to assess it TODO

24.2 What it does

TODO

24.3 When to do it

TODO

24.4 How to do it

TODO

24.5 How to assess it

Bibliography

Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani. *An Introduction to Statistical Learning*. Springer, 2nd edition, 2021. URL https://link.springer.com/book/10.1007/978-1-0716-1418-1. ISBN 978-1-0716-1417-4.