

# Regularized Logistic Regression

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# 1. Logistic Regression

Logistic regression is a key model.

It allows us to use ideas from linear modeling to predict a binary outcome.

The model is:

$$P(Y = 1 | x) = F(x'\beta), \quad F(\eta) = \frac{e^\eta}{1 + e^\eta} = \frac{1}{1 + e^{-\eta}}.$$

As in linear regression,  $x'\beta$  is a linear combination of the features which may include a 1 for an intercept.

$$x'\beta = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p.$$

Note that  $F : R \rightarrow (0, 1)$ .

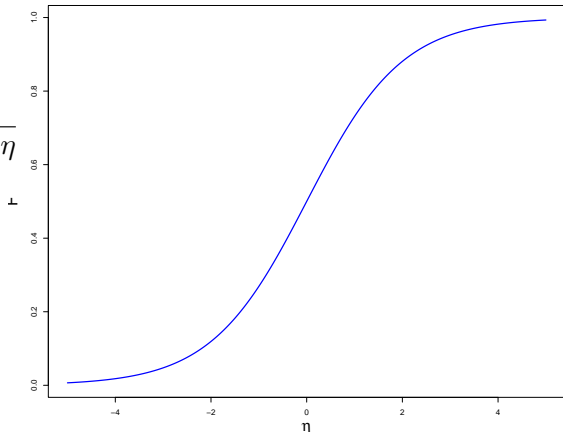
$F$  is called the logistic function or the sigmoid function.

The logistic function:

$$\begin{aligned} F(\eta) &= \frac{e^\eta}{1 + e^\eta} \\ &= \frac{1}{1 + e^{-\eta}} \end{aligned}$$

The key idea is that  $F(\eta)$  is always between 0 and 1 so we can use it as a probability.

Note that  $F$  is increasing, so if  $\eta$  goes up  $F(\eta)$  goes up.



$$F(-3) = .05, F(-2) = .12, F(-1) = .27$$

$$F(0) = .5$$

$$F(1) = .73, F(2) = .88, F(3) = .95$$

## Log Odds

Our model is:

$$p(Y = 1 | x, \beta) = \frac{e^{x'\beta}}{1 + e^{x'\beta}}.$$

So,

$$\log\left(\frac{p(Y = 1 | x, \beta)}{1 - p(Y = 1 | x, \beta)}\right) = x' \beta.$$

The log of the odds ratio  $Y=1$  vs  $Y=0$ , is linear in  $x$ .

For example:

$$P(Y = 1 | x, \beta) = .5 \iff \log \text{ odds} = 0 \iff x' \beta = 0.$$

Let's use the Default data (from the ISLR book):

```
> library(ISLR2)
> data(Default)
> summary(Default)
```

| default  | student  | balance        | income        |
|----------|----------|----------------|---------------|
| No :9667 | No :7056 | Min. : 0.0     | Min. : 772    |
| Yes: 333 | Yes:2944 | 1st Qu.: 481.7 | 1st Qu.:21340 |
|          |          | Median : 823.6 | Median :34553 |
|          |          | Mean : 835.4   | Mean :33517   |
|          |          | 3rd Qu.:1166.3 | 3rd Qu.:43808 |
|          |          | Max. :2654.3   | Max. :73554   |

Each observation corresponds to an account.

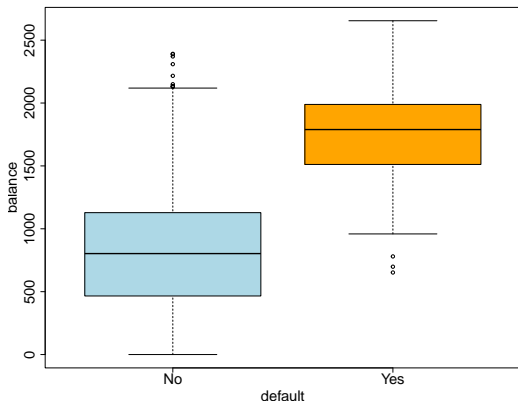
Our “y” is the binary “ do they default”. x is things about the account.

## Quick look at the data.

Divide the data into two groups, one group has  $y=No$  and other other group has  $y=Yes$ .

Use boxplots to display the  $x=balance$  values in each subgroup.

The balance values are bigger for the default  $y=Yes$  observations!



## The Default Data, Logistic Regression with MLE

Here is the logistic regression output using all three  $x$ 's in the data set: balance, income, and student.

student is coded up as a factor, so R automatically turns it into a dummy.

Call:

```
glm(formula = default ~ balance + student + income, family = binomial,
    data = Default)
```

Deviance Residuals:

| Min     | 1Q      | Median  | 3Q      | Max    |
|---------|---------|---------|---------|--------|
| -2.4691 | -0.1418 | -0.0557 | -0.0203 | 3.7383 |

Coefficients:

|             | Estimate   | Std. Error | z value | Pr(> z )    |
|-------------|------------|------------|---------|-------------|
| (Intercept) | -1.087e+01 | 4.923e-01  | -22.080 | < 2e-16 *** |
| balance     | 5.737e-03  | 2.319e-04  | 24.738  | < 2e-16 *** |
| studentYes  | -6.468e-01 | 2.363e-01  | -2.738  | 0.00619 **  |
| income      | 3.033e-06  | 8.203e-06  | 0.370   | 0.71152     |

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 2920.6 on 9999 degrees of freedom  
Residual deviance: 1571.5 on 9996 degrees of freedom  
AIC: 1579.5

Number of Fisher Scoring iterations: 8

Note:

Number of Fisher Scoring iterations: 8

The estimates are MLE.

The maximization uses Newton's method which is an iterative procedure.

*It took 8 iterations for the maximization to converge !!!*

The estimates are MLE.

Confidence intervals are estimate +/- 2 standard errors.

e.g for studentYes coefficient :  $-.65 \pm 2(.24) = -.65 \pm .5$

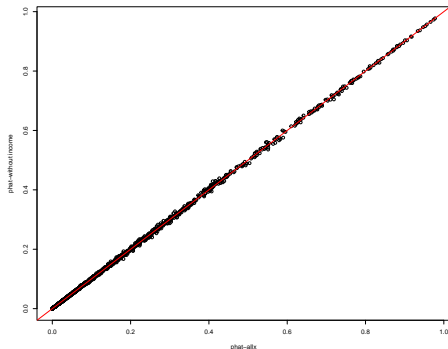
Z-stats are (estimate-proposed)/se.

To test whether the coefficient for income is 0, we have  $z = (3.033-0)/8.203 = .37$ , so we fail to reject.

The p-value is  $2*P(Z < -.37) = 2*pnorm(-.37) = 0.7113825$ .

So, the output suggests we may not need `income`.

Here is a plot of the fitted probabilities with and without `income` in the model.



We get almost the same probabilities, so, as a practical matter, `income` does not change the fit.

Here is the output using balance and student.

Call:

```
glm(formula = default ~ balance + student, family = binomial,  
     data = Default)
```

Deviance Residuals:

|  | Min     | 1Q      | Median  | 3Q      | Max    |
|--|---------|---------|---------|---------|--------|
|  | -2.4578 | -0.1422 | -0.0559 | -0.0203 | 3.7435 |

Coefficients:

|             | Estimate   | Std. Error | z value | Pr(> z )     |
|-------------|------------|------------|---------|--------------|
| (Intercept) | -1.075e+01 | 3.692e-01  | -29.116 | < 2e-16 ***  |
| balance     | 5.738e-03  | 2.318e-04  | 24.750  | < 2e-16 ***  |
| studentYes  | -7.149e-01 | 1.475e-01  | -4.846  | 1.26e-06 *** |

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 2920.6 on 9999 degrees of freedom  
Residual deviance: 1571.7 on 9997 degrees of freedom  
AIC: 1577.7

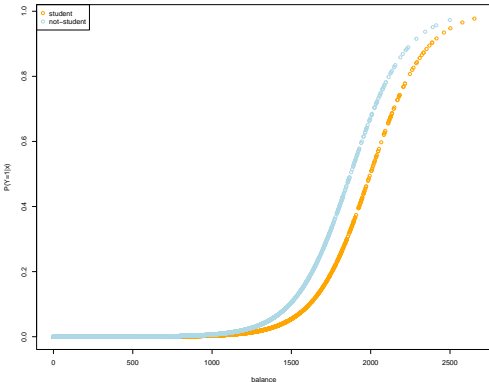
Number of Fisher Scoring iterations: 8

$$P(Y = 1 \mid x = (\text{balance}, \text{studentYes})) = F(-1.075 + .005738 \text{ balance} - .7149 \text{ studentYes})$$

With just `balance` and `student` in the model, we can plot  $P(Y = 1 \mid x)$  vs.  $x$ .

The orange points are for the students and the blue are for the non-students.

In both cases the probability of default increases with the balance, but at any fixed balance, a student is less likely to default.



## AIC and BIC in Logistic Regression

In the logistic regression model, the *deviance* is just -2 times the logLikelihood (usually evaluated at the mle).

$$L(\beta) = \prod_{i=1}^n P(Y = y_i | X = x_i, \beta)$$

For logistic regression,  $P(Y = 1 | x, \beta) = F(x'\beta)$ ,  $F(\eta) = \frac{\exp(\eta)}{(1 + \exp(\eta))}$ .

Given an estimate (usually a MLE)  $\hat{\beta}$ ,

$$deviance = -2 \sum_{i=1}^n \log(P(Y = y_i | X = x_i, \hat{\beta}))$$

The better the fit of the model, the bigger the likelihood, the smaller the deviance.

## AIC:

AIC is the deviance + a model complexity penalty term.

$$AIC = deviance + 2 * (p + 1)$$

We penalize our fit as measured by the deviance with a penalty of 2 for each parameter.

Here we assume our parameters are  $p$  slopes for  $p \times$  features + 1 intercept giving  $p + 1$ .

We like the model with a small AIC, good fit as measured by the deviance but not too complex.

## AIC for the Default example:

With balance+student we had:

Residual deviance: 1571.7 on 9997 degrees of freedom

AIC: 1577.7

A parameter (a coefficient) costs 2.

- ▶ balance + student:

Residual deviance: 1571.7, AIC:  $1577.7 = 1571.7 + 2*(3)$ .

- ▶ balance:

Residual deviance: 1596.5, AIC:  $1600.5 = 1593.5 + 2*(2)$ .

- ▶ balance + student + income:

Residual deviance: 1571.5, AIC:  $1579.5 = 1571.5 + 2*(4)$ .

- ▶ student:

Residual deviance: 2908.7, AIC:  $2912.7 = 2908.7 + 2*(2)$ .

⇒ pick balance+student

BIC:

BIC is an alternative to AIC, but the penalty is different.

$$BIC = deviance + \log(n) * (p + 1)$$

$\log(n)$  tends to be bigger than 2, so BIC has a bigger penalty, so it suggest smaller models than AIC.

## BIC for the Default example:

$$\log(10000) = 9.21034.$$

A parameter (a coefficient) costs 9.2.

- ▶ balance:  
1596.5, BIC:  $= 1593.5 + 9.2*(2) = 1611.9.$
- ▶ balance + student + income:  
BIC:  $= 1571.5 + 9.2*(4) = 1608.3.$
- ▶ balance + student:  
BIC:  $= 1571.7 + 9.2*(3) = 1599.3.$
- ▶ student:  
BIC:  $= 2908.7 + 9.2*(2) = 2927.1.$

⇒ pick balance+student

Which is better, AIC or BIC??

*nobody knows.*

R prints out AIC, which suggests you might want to use it, but a lot of people like the fact that BIC suggests simpler models.

A lot of academic papers report both AIC and BIC and if they pick the same model are happy with that. Lame.

*Checking the out of sample performance is safer !!!*

## 2. The Logistic Likelihood

We have a very general intuition that we can use the negative log likelihood as a measure of fit on training data.

In linear regression with iid normal errors, we saw that the form of the log likelihood is very intuitive in terms of the error sum of squares.

In the linear case, minimizing the log likelihood is the least squared problem and the LASSO could be written

$$\underset{\beta}{\text{minimize}} \quad -\log(L(\beta)) + \lambda \sum_{j=1}^p |\beta_j|.$$

We follow exactly this approach for logistic regression.

But, let's have a closer look at the log likelihood and see if it is intuitive!!

For logistic regression we have:

$$P(y_i | x_i, \beta) = \begin{cases} F(x_i^T \beta) & y_i = 1 \\ 1 - F(x_i^T \beta) & y_i = 0 \end{cases} \quad F(\eta) = \frac{e^\eta}{1 + e^\eta}$$

$$L(\beta) = \prod_{i=1}^n P(y_i | x_i, \beta)$$

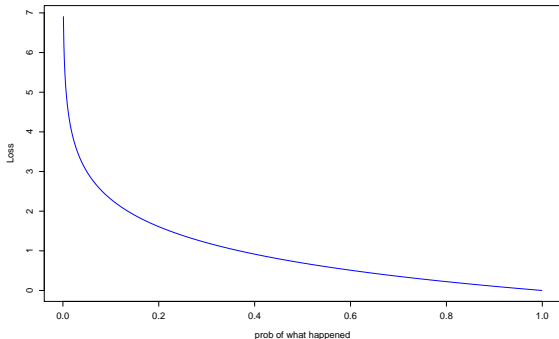
$$\begin{aligned} -\log L(\beta) &= \sum_{i=1}^n -\log(P(y_i | x_i, \beta)) \\ &= \sum_{i=1}^n -\log(\text{probability of what happened}) \end{aligned}$$

So, for an individual observation the contribution is  $-\log(\text{prob of what happened})$ .

x axis: probability of what happened (according to your model).

y axis: your loss.

In our logit problem “what happened” is either a 0 or a 1.



If your model gives a high probability to what happened, you have a small loss.

If your model gives a low probability to what happened, you have a big loss.

### 3. L2 and L1 Regularized Logistic Regression

For linear models, we found that regularized versions gave us a very nice way to explore the bias-variance tradeoff.

We added a penalty term whose weighting parameter  $\lambda$  controlled the extent to which the coefficients were shrunk towards 0.

We would like to be able to do the same thing with logistic regression.

We want *regularized logistic regression*.

## L2:

To get the ridge regression of logistic regression we just add the L2 penalty:

$$\underset{\beta}{\text{minimize}} \quad -\log(L(\beta)) + \frac{\lambda}{2} \sum \beta_j^2$$

## L1:

To get the Lasso regression of logistic regression we just add the L1 penalty:

$$\underset{\beta}{\text{minimize}} \quad -\frac{1}{n} \log(L(\beta)) + \lambda \sum |\beta_j|$$

As in our discussion of the deviance,  $-\log(L(\beta))$  is a measure of fit on the training data.

Big  $L$  means good fit, so small  $-\log(L(\beta))$  means good fit.

## 4. Simulated Example

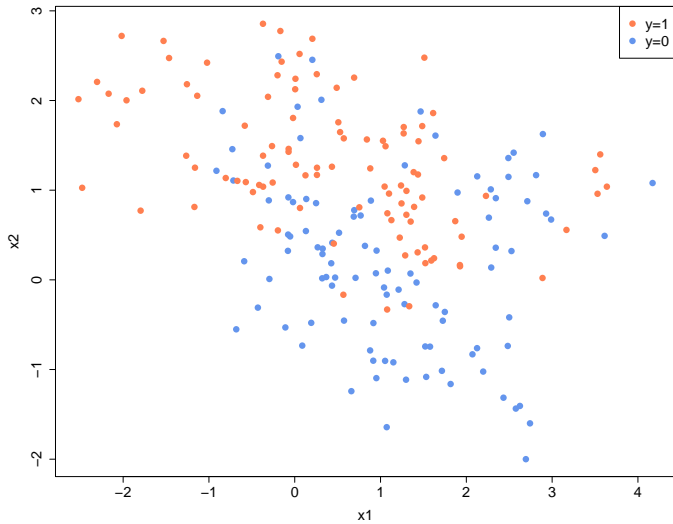
Let's look at a simulated example from the “Elements of Statistical Learning” (`library(ElmStatLearn)`) R package.

*Description*

*This is a simulated mixture example with 200 instances and two classes. 100 members in each class.*

We have two numeric  $x$ 's creatively called  $x_1$  and  $x_2$  and one binary outcome  $y$ .

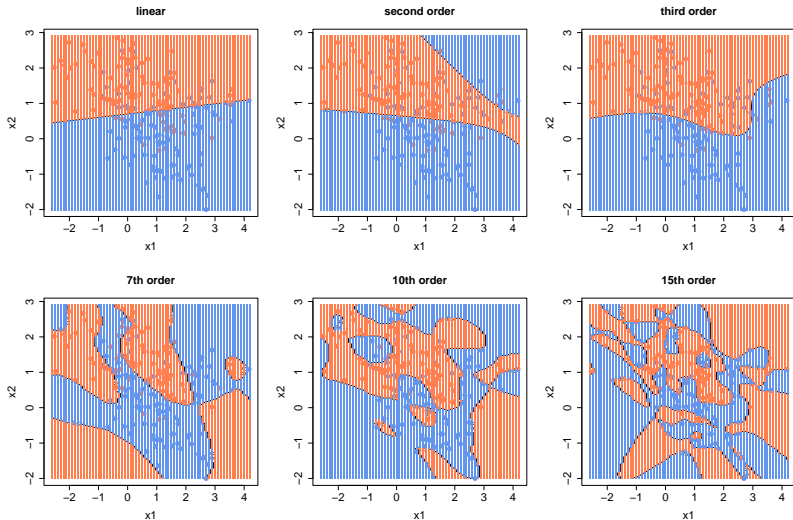
Plot the data: two numeric  $x$  and a binary  $y$ .



Now let's run logistic regression so  $y$  on  $x$ , throwing in more and more polynomials in  $x_1$  and  $x_2$ .

We use the R function `poly` to construct all the polynomials.

Decision Boundary plots of logit fits with varying degrees of polynomial terms thrown in.



*which one do you like the best ???*

Ok, now let's try the Lasso.

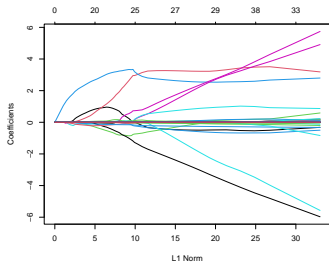
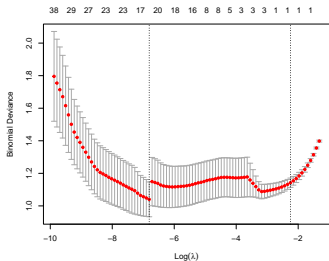
We will throw in all the 15th order terms.

This gives us 135  $x$ 's !!!!!!!

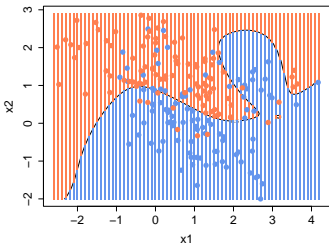
```
> 15*14/2 + 2*15  
[1] 135
```

Of course, the fit using all of these is overfit.

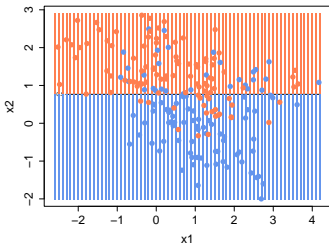
But, can we use the Lasso to explore the possibility that some subset of the 135 is good?



**Lasso: min lambda decision boundary**



**Lasso: min lambda 1se decision boundary**



Both of these look reasonable.

We got to try using all 135  $x$ 's, but the cv process pulls us back to something more restrained.

What transformations did the Lasso choose?

Here are the non-zero coefficients from lambda.min.

|               |               |              |               |               |
|---------------|---------------|--------------|---------------|---------------|
| (Intercept)   | x.1.0         | x.2.0        | x.3.0         | x.7.0         |
| -2.495723e+00 | 9.241824e-01  | 1.000302e+00 | -4.584982e-01 | 1.136215e-03  |
| x.8.0         | x.15.0        | x.0.1        | x.3.1         | x.2.2         |
| 1.362927e-04  | -3.150041e-08 | 2.922533e+00 | -4.609735e-02 | -2.478831e-01 |
| x.3.2         | x.8.2         | x.1.3        | x.7.3         | x.8.3         |
| -1.885774e-01 | 3.671665e-04  | 7.296183e-02 | 1.149181e-04  | 1.348425e-04  |
| x.0.4         | x.2.7         | x.0.15       |               |               |
| -1.329917e-01 | 4.745585e-03  | 1.255572e-06 |               |               |

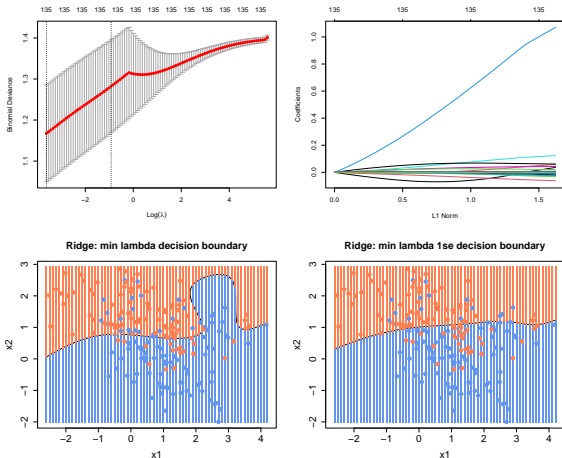
Wow,  $x_1^8 \times x_3^2$  comes in, not obvious!!

Here are the non-zero coefficients from lambda.1se.

|             |           |
|-------------|-----------|
| (Intercept) | x.0.1     |
| -0.5352522  | 0.6994122 |

And the simple model is just use  $x_2$  which is clearly a reasonable choice give the plot of the data.

Here are the results for Ridge regression.



What  $x$  do you think the big coefficient is for?

Note that the default choice of  $\lambda$  grid does not give us the bottom of the U.

Here are the largest absolute values of the Ridge coefficients at  $\lambda_{\min}$ .

|                   |             |             |             |             |             |
|-------------------|-------------|-------------|-------------|-------------|-------------|
| x.0.1 (Intercept) |             | x.1.1       | x.1.2       | x.0.2       | x.2.0       |
| 1.070560515       | 0.856423790 | 0.123268634 | 0.061601542 | 0.061160591 | 0.058390390 |
| x.2.1             | x.1.0       | x.2.2       | x.3.0       | x.3.2       | x.0.3       |
| 0.043099658       | 0.036520614 | 0.032405780 | 0.024975048 | 0.022550293 | 0.020280928 |
| x.3.1             | x.0.4       | x.1.3       | x.3.3       | x.0.5       | x.3.4       |
| 0.018121108       | 0.009203506 | 0.008768088 | 0.006534978 | 0.003175778 | 0.003083115 |
| x.4.2             | x.2.3       |             |             |             |             |
| 0.002955913       | 0.002828573 |             |             |             |             |

So,  $x_2$  (same as x.0.1) dominates the fit.

## 5. We8There

Each observation consists of a restaurant review.

We also have the Zagat ratings for each restaurant.

We want to see how the Zagat rating relates to reviews.

What kind of customer review correspond to a good rating?

We have 6,166 observations.

Here are the Zagat ratings summarized:

| 1   | 2   | 3   | 4    | 5    |
|-----|-----|-----|------|------|
| 615 | 493 | 638 | 1293 | 3127 |

We will dichotomize the outcome by making  $y$  1 if the overall rating is greater than 3 and 0 otherwise.

| $y$ | 0    | 1    |
|-----|------|------|
|     | 1746 | 4420 |

What is our  $x$ ?

We want to use the information in the text of the restaurant reviews.

How do we convert the text of a review into a numeric  $x$ ??

## Bag of Words:

The most common way to look at a text document is to treat it as a bag of words.

That is, we look all the words in all the documents and then make a list of words or “terms” of interest.

For example the word “the” will probably occur with some frequency, but that may not be deemed to be of interest.

Given the list of terms, we just count the number of times each term occurs in the text of the document.

Note that this approach ignores the *word order*, the document is treated as a “bag of words”.

## bigrams:

A bi-gram is just a pair of words appearing in sequence.

For example, the pair of words “good food” appearing in sequence may mean more than “good” or “food” by themselves.

We will make a list of bigrams and then  $x$  will be the number of times each bigram occurs in the text of a review.

The dimension of our  $X$  matrix is:

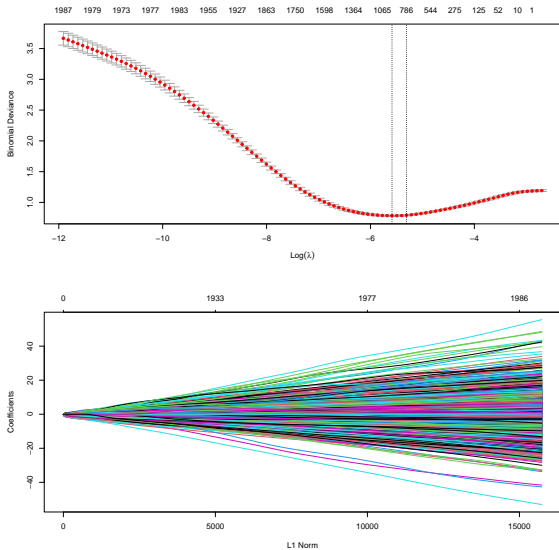
```
[1] 6166 2640
```

There are 2,640 bigrams in our list of ones we are counting.

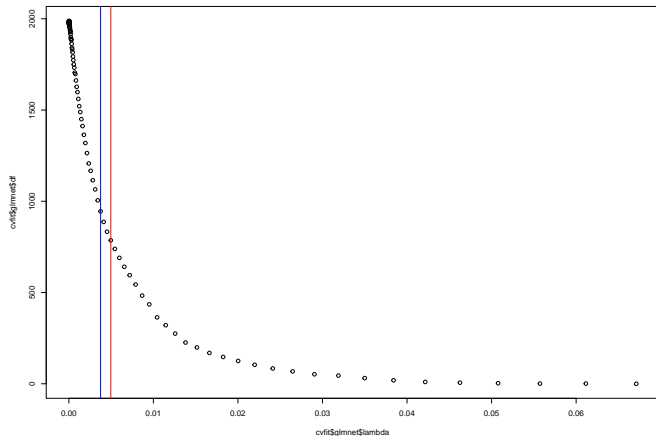
In our first observation, the bigrams with a non-zero count are:

```
even though larg portion  mouth water      red sauc    babi back    back rib
      1              1              1              1              1              1
chocol mouss veri satisfi
      1              1
```

Here is the Lasso fit:



Here is the number of non-zero coefficients plotted against  $\lambda$ .



Lines drawn at `lambda.min` and `lambda.1se`.

# Here are the big positive and big negative coefficients.

## Big positive coefficients:

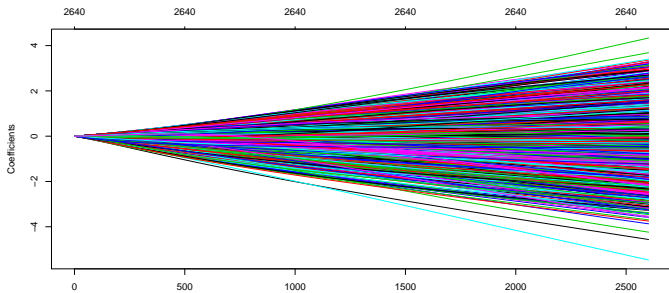
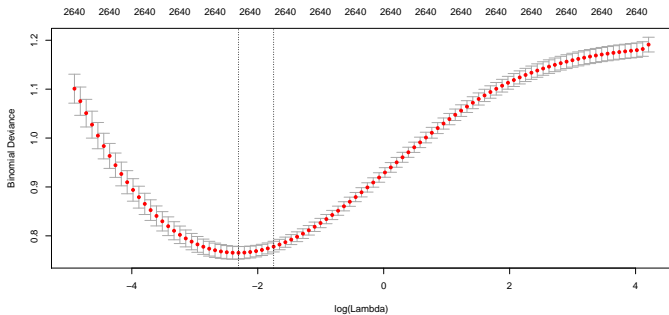
|      |                |                 |                     |           |           |           |           |
|------|----------------|-----------------|---------------------|-----------|-----------|-----------|-----------|
| [1]  | "between two"  | "can wait"      | "beef sandwich"     |           |           |           |           |
| [4]  | "friend help"  | "best meal"     | "high recommend"    |           |           |           |           |
| [7]  | "cannot wait"  | "melt mouth"    | "food delici"       |           |           |           |           |
| [10] | "portion huge" | "wonder experi" | "veri unigu"        |           |           |           |           |
| [13] | "pretti quick" | "can beat"      | "full bar"          |           |           |           |           |
| [16] | "look out"     | "absolut best"  | "definit recommend" |           |           |           |           |
| [19] | "(Intercept)"  | "now live"      | "quit few"          |           |           |           |           |
| [22] | "well worth"   | "better most"   | "never bad"         |           |           |           |           |
| [25] | "out world"    | "great food"    | "wall cover"        |           |           |           |           |
| [28] | "up good"      | "great experi"  | "absolut delici"    |           |           |           |           |
| [1]  | 1.6235758      | 1.3860122       | 1.3672099           | 1.3413956 | 1.2976254 | 1.2863832 | 1.1719763 |
| [8]  | 1.1502664      | 1.1288480       | 1.1032885           | 1.0835135 | 1.0807977 | 1.0533985 | 1.0492868 |
| [15] | 1.0435863      | 1.0429624       | 1.0308216           | 0.9933000 | 0.9842953 | 0.9840952 | 0.9834227 |
| [22] | 0.9633459      | 0.9578412       | 0.9512289           | 0.9375038 | 0.9236589 | 0.9104929 | 0.9073509 |
| [29] | 0.9026439      | 0.8981764       |                     |           |           |           |           |

## Big negative coefficients:

|      |                |                   |                  |                  |           |           |           |
|------|----------------|-------------------|------------------|------------------|-----------|-----------|-----------|
| [1]  | "over cook"    | "waitress seem"   | "just ok"        | "bad food"       |           |           |           |
| [5]  | "food poison"  | "servic ok"       | "servic slow"    | "mediocr food"   |           |           |           |
| [9]  | "one worst"    | "wast money"      | "food okay"      | "mani option"    |           |           |           |
| [13] | "anoth chanc"  | "veri disappoint" | "food averag"    | "terribl servic" |           |           |           |
| [17] | "veri slow"    | "veri poor"       | "veri bland"     | "quick lunch"    |           |           |           |
| [21] | "never go"     | "gone down"       | "servic terribl" | "food terribl"   |           |           |           |
| [25] | "never return" | "stay away"       | "far better"     | "mediocr best"   |           |           |           |
| [29] | "veri rude"    | "extrem rude"     |                  |                  |           |           |           |
| [1]  | -1.484979      | -1.501437         | -1.526967        | -1.528732        | -1.540570 | -1.569690 | -1.585480 |
| [8]  | -1.591799      | -1.642964         | -1.652540        | -1.672776        | -1.673099 | -1.685418 | -1.704577 |
| [15] | -1.752020      | -1.770758         | -1.780688        | -1.792626        | -1.803219 | -1.831518 | -1.899799 |
| [22] | -2.025952      | -2.035374         | -2.044341        | -2.087831        | -2.097159 | -2.267862 | -2.277634 |
| [29] | -2.322275      | -2.524030         |                  |                  |           |           |           |

Not surprising that it is bad to be "extrem rude".

Here are Ridge results.



Big positive coefficients:

|      |                  |                  |                |                  |           |           |           |
|------|------------------|------------------|----------------|------------------|-----------|-----------|-----------|
| [1]  | "(Intercept)"    | "coconut shrimp" | "look out"     | "veri uniqu"     |           |           |           |
| [5]  | "year food"      | "servic attent"  | "friend help"  | "well food"      |           |           |           |
| [9]  | "everyth menu"   | "half shell"     | "veri cozi"    | "absolut best"   |           |           |           |
| [13] | "absolut delici" | "serv hot"       | "staff make"   | "same peopl"     |           |           |           |
| [17] | "fair price"     | "can beat"       | "between two"  | "excel price"    |           |           |           |
| [21] | "salad great"    | "cannot wait"    | "restaur make" | "time re"        |           |           |           |
| [25] | "back home"      | "best meal"      | "food superb"  | "thorough enjoy" |           |           |           |
| [29] | "reserv suggest" | "keep go"        |                |                  |           |           |           |
| [1]  | 0.9126494        | 0.6568706        | 0.6541469      | 0.6532986        | 0.6495907 | 0.6485409 | 0.6415978 |
| [8]  | 0.6413095        | 0.6396719        | 0.6378453      | 0.6257804        | 0.6232927 | 0.6146492 | 0.6085780 |
| [15] | 0.6063171        | 0.6015257        | 0.6008904      | 0.5989794        | 0.5986393 | 0.5957714 | 0.5942530 |
| [22] | 0.5889521        | 0.5856139        | 0.5836239      | 0.5766060        | 0.5764588 | 0.5733635 | 0.5724580 |
| [29] | 0.5715484        | 0.5708517        |                |                  |           |           |           |

Big negative coefficients:

|      |                   |                  |                  |               |            |            |  |
|------|-------------------|------------------|------------------|---------------|------------|------------|--|
| [1]  | "one worst"       | "anoth chanc"    | "just anoth"     | "day befor"   |            |            |  |
| [5]  | "veri disappoint" | "quick lunch"    | "food mediocr"   | "veri poor"   |            |            |  |
| [9]  | "wast money"      | "servic slow"    | "terribl servic" | "servic ok"   |            |            |  |
| [13] | "got bill"        | "stay away"      | "food terribl"   | "mani option" |            |            |  |
| [17] | "veri limit"      | "servic terribl" | "complain manag" | "veri bland"  |            |            |  |
| [21] | "just ok"         | "mediocr food"   | "food averag"    | "veri rude"   |            |            |  |
| [25] | "food okay"       | "veri slow"      | "mediocr best"   | "gone down"   |            |            |  |
| [29] | "far better"      | "extrem rude"    |                  |               |            |            |  |
| [1]  | -0.8566305        | -0.8635339       | -0.8699492       | -0.8787698    | -0.8881075 | -0.8920423 |  |
| [7]  | -0.9201352        | -0.9373039       | -0.9438574       | -0.9541782    | -0.9581192 | -0.9590981 |  |
| [13] | -0.9771998        | -0.9841832       | -0.9843469       | -0.9920617    | -1.0010190 | -1.0014385 |  |
| [19] | -1.0104797        | -1.0179680       | -1.0222027       | -1.0260030    | -1.0503238 | -1.0819638 |  |
| [25] | -1.0859973        | -1.0939149       | -1.1249573       | -1.1382567    | -1.2025776 | -1.2955933 |  |

## 6. Multinomial Logit

The problem where  $Y$  is a binary outcome is very common.

But how do we extend logistic regression to the multinomial outcome case?

Let's look at the forensic glass data and use two of the  $x$ 's (so we can plot) and all three of the outcomes.

## Example, Forensic Glass:

*Can you tell what kind of glass it was from measurements on the broken shards??*

**Y: glass type, 3 categories.**

$Y \in S = \{\text{WinF}, \text{WinNF}, \text{Other}\}.$

WinF: float glass window

WinNF: non-float window

Other.

**x: 3 numeric x's:**

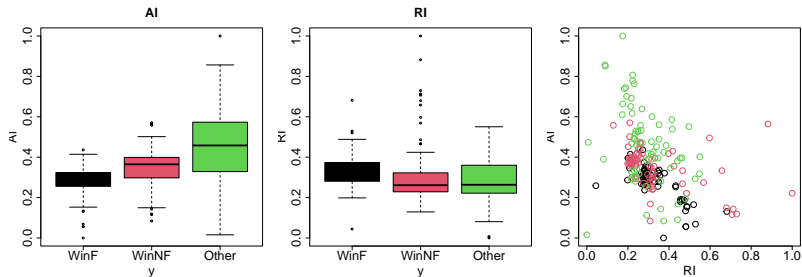
$x_1 = \text{RI: refractive index}$

$x_2 = \text{Al}$

$x_3 = \text{Na}$

Let's use two of the  $x$ 's (so we can plot) and all three of the outcomes.

Here is the three outcome  $Y$  plotted against the two  $x$ 's  $x=(RI,AI)$ .



## kNN:

Before we go into the linear multinomial model, let's just note that KNN for classification is obvious.

Given test  $x$  and training  $(x_i, y_i)$ :

*Numeric Y:*

- ▶ find the  $k$  training observations with  $x_i$  closest to  $x$ .
- ▶ predict  $y$  with the average of the  $y$  values for the neighbors.

*Categorical Y:*

- ▶ find the  $k$  training observations with  $x_i$  closest to  $x$ .
- ▶ predict  $Y$  with the most frequent of the  $y$  values for the neighbors.
- ▶ estimate  $P(Y = y | x)$  with the proportion of neighbors having  $Y = y$ .

## Multinomial Logit:

The multinomial logit model for  $Y \in \{1, 2, \dots, C\}$  is

$$P(Y = j|x) \propto \exp(x'\beta_j), \quad j = 1, 2, \dots, C.$$

Or,

$$P(Y = j|x) = \frac{\exp(x'\beta_j)}{\sum_{j=1}^C \exp(x'\beta_j)}$$

*So, each category gets a linear (affine) function of  $x$  !!!*

## Softmax Function:

For  $x = (x_1, x_2, \dots, x_C)$  The softmax function is

$$\sigma(x)_j = \frac{e^{x_j}}{\sum_j e^{x_j}}$$

Exponentiate and then normalize.

Takes a vector of real numbers  $x_j$  and maps them to a probability vector.

We use this a lot.

## Identification:

Suppose we add  $\beta$  to each  $\beta_j$ .

$$\begin{aligned}P(Y = j|x) &= \frac{\exp(x'(\beta_j + \beta))}{\sum \exp(x'(\beta_j + \beta))} \\ &= \frac{\exp(x'\beta) \exp(x'\beta_j)}{\exp(x'\beta) \sum \exp(x'\beta_j)} \\ &= \frac{\exp(x'\beta_j)}{\sum \exp(x'\beta_j)}\end{aligned}$$

So, if we add any vector to all the  $\beta_j$  we get the exact same model!!

In this case we say the set of parameters  $\{\beta_j\}$  is not identified in that two different sets can give you the exact same likelihood.

The common identification strategy is to pick one of the  $\beta_j$  and set it equal to 0. Usually, it is either the “first” or the “last”  $\beta_j$ .

Note that as usual  $x$  may be  $(1, x_2, \dots, x_p)'$ , that is we have included an intercept.

Here is output from fitting a multinomial logit using the forensic glass data.

( R package nnet, function multinom).

Call:

```
multinom(formula = y ~ ., data = ddf, maxit = 1000)
```

Coefficients:

|       | (Intercept) | RI       | Al        |
|-------|-------------|----------|-----------|
| WinNF | -3.277900   | 2.819056 | 7.861631  |
| Other | -5.651027   | 2.718534 | 13.616921 |

Std. Errors:

|       | (Intercept) | RI       | Al       |
|-------|-------------|----------|----------|
| WinNF | 1.030785    | 1.610635 | 2.049922 |
| Other | 1.165932    | 1.872040 | 2.263372 |

Residual Deviance: 402.6627

AIC: 414.6627

The first  $\beta$  has been set to 0.

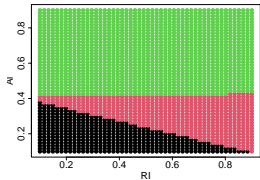
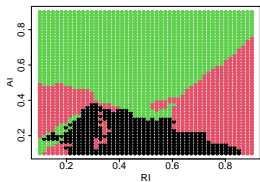
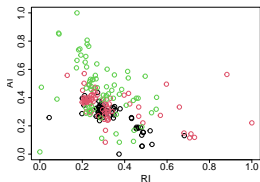
Note:  $402.6627 + 12 = 414.6627$

plot of the data.

The color indicates the most probable outcome. black=WinF, red=WinNF, green=Other.

Most probable from knn.  
k=20.

Most probable from multinomial logit.



So, all but one class gets it's own coefficient vector.

Coefficients:

|       | (Intercept) | RI       | AI        |
|-------|-------------|----------|-----------|
| WinNF | -3.277900   | 2.819056 | 7.861631  |
| Other | -5.651027   | 2.718534 | 13.616921 |

```
> table(y)
```

```
y
  WinF WinNF Other
    70    76    68
```

The coefficient vector for WinF has been set to 0.

$\beta_1 = (0.0, 0)$ , for WinF

$\beta_2 = (-3.277900, 2.819056, 7.861631)$ , for WinNF.

$\beta_3 = (-5.651027, 2.718534, 13.616921)$ , for Other.

Let

$$\eta_1 = 0$$

$$\eta_2 = -3.28 + 2.82RI + 7.86AI$$

$$\eta_3 = -5.65 + 2.72RI + 13.62AI$$

$$P(Y = \text{WinF} = 1|x) = \frac{1}{1 + e^{\eta_2} + e^{\eta_3}}$$

$$P(Y = \text{WinNF} = 2|x) = \frac{e^{\eta_2}}{1 + e^{\eta_2} + e^{\eta_3}}$$

$$P(Y = \text{Other} = 3|x) = \frac{e^{\eta_3}}{1 + e^{\eta_2} + e^{\eta_3}}$$

When both AI and RI are small, the negative intercepts mean  $Y=\text{WinF}=1$  is more likely.

When AI increases,  $Y=\text{Other}$ , becomes much more likely because of the large 13.62 coefficient.