THE UNIVERSITY OF TEXAS AT AUSTIN

McCOMBS BUSINESS ANALYTICS

Classification: Logistic Regression and Naive Bayes

Book Chapter 4.

Carlos M. Carvalho
The University of Texas McCombs School of Business

1. Classification

When the y we are trying to predict is *categorical* (or *qualitative*), we say we have a *classification* problem.

For a numeric (or *quantitative*) y we predict it's value.

For a categorical y we try to guess which of a listed number of possible outcomes will happen.

The basic case is a binary y: something will either happen or not.

We have already seen classification in our introductory section using KNN where the response was the type of glass and x was characteristics of the glass shard.

Classification

There are a large number of methods for classification.
We have seen KNN.

In this section of notes we will learn about logistic regression and naive Bayes.

Later, we will study trees, Random Forests, and boosting, which are also important classification methods.

Classification

Some classification methods just try to assign a y to a category given x.

In this section of notes we study two techniques which take a probabilistic view and try to come up with:

$$Pr(Y = y \mid X = x)$$

the probability the Y ends up having class label y given the information in x.

Classification

$$Pr(Y = y \mid X = x)$$

Logistic Regression:

Estimates $Pr(Y = y \mid X = x)$ directly.

Naive Bayes:

Comes up with

- $p(Y = y)$ (the marginal for Y)
- $P(X = x \mid Y = y)$ (the conditional distribution of X given Y)

and then uses Bayes Theorem to compute $P(Y = y \mid X = x)$.

Classification

In section 10 we will review Bayes Theorem and some basic probability ideas we have used informally.

In section 7 we will look at decision theory and loss in more detail. We have already made extensive use of the idea of a loss function, but now add another layer which plays an important role in classification.

2. Logistic Regression, One Predictor

To start off as simply as possible, we will first consider the case where we have a binary y and one numeric x.

Lets' look at the Default data (from Chapter 4):

- y:
  whether or not a customer defaults on their credit card (No or Yes).

- x:
  The average balance that the customer has remaining on their credit card after making their monthly payment.

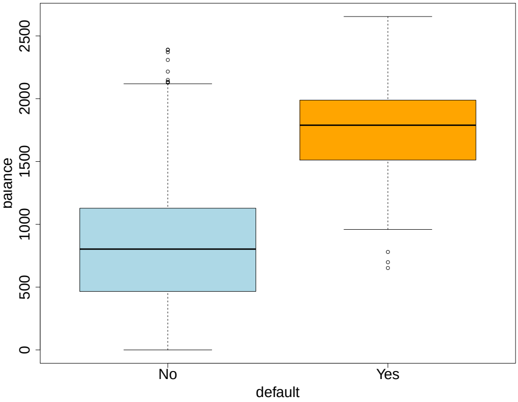
- 10,000 observations, 333 defaults (.0333 default rate).

Let's 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!



In our example, we would want

$$Pr(Y = Yes \mid X = x).$$

Given the probability we can classify using a rule like

$$\text{guess Yes } \textit{if}\text{: } Pr(Y = Yes \mid x) > .5.$$

Notation:

For a binary y, it is very common to use a dummy variable to code up the two possible outcomes.

So, in our example, we might say a default means $Y = 1$ and a non-default means $Y = 0$.

In the context of an example we might use the label and $Y = 1$ interchangeably.
In our default example, $P(Y = 1 \mid X = x)$ and $P(Y = yes \mid X = x)$ would mean the same thing.

Normally, we might use names like D and B for our two variables, but since we want to think about the ideas in general, let's stick with Y and X.

Logistic regression uses the power of linear modeling and estimates $Pr(Y = y \mid x)$ by using a two step process.

- Step 1:

  apply a linear function to x: $x \rightarrow \eta = \beta_0 + \beta_1 x$.

- Step 2:

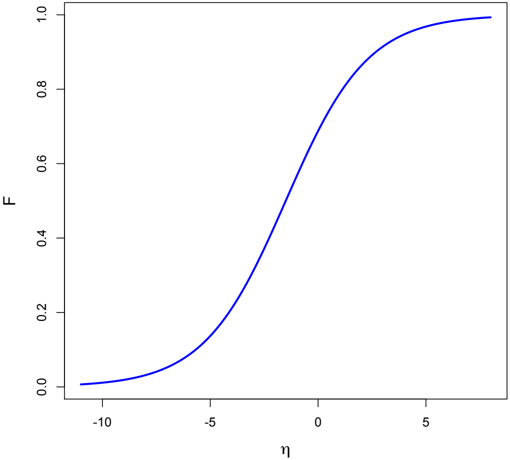
  apply the *logistic function* F,
  to η to get a number between 0 and 1.
  $P(Y = 1 \mid x) = F(\eta)$.

The logistic function:

$$F(\eta) = \frac{e^{\eta}}{1 + e^{\eta}}.$$

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 η goes up $P(Y = 1 \mid x)$ goes up.



$$F(-3) = .05,\ F(-2) = .12,\ F(-1) = .27,\ F(0) = .5$$

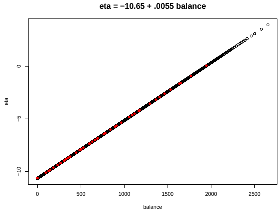
$$F(0) = .5$$

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

Logistic fit to the y=default, x=balance data.

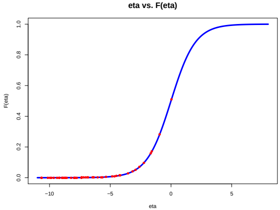
First, logistic looks for a linear function of x it can feed into the logistic function.

Here we have
$\eta = -10.65 + .0055\,x$.

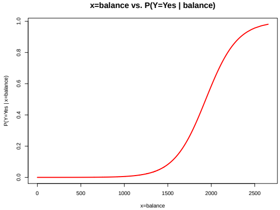


Next we feed the η values into the logistic function.

100 randomly sampled observations are plotted with red dots.



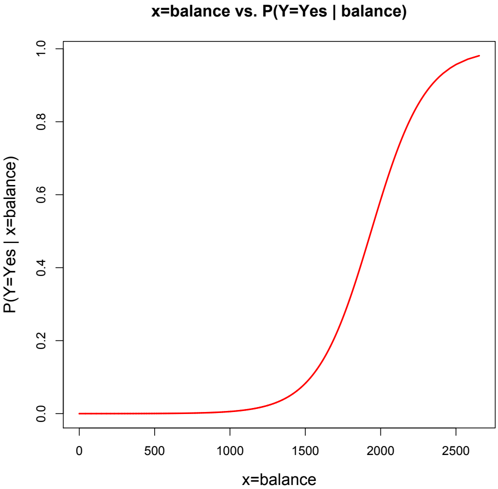
We can combine the two steps together and plot
x=balance vs.
$P(Y = Yes \mid x) = F(-10.65 + .0055\,x)$.



Logistic Regression:

Combining the two steps, our logistic regression model is:

$$P(Y = 1 \mid X = x) = F(\beta_0 + \beta_1 x).$$



3. Inference: Esimtating the Parameters

Logistic regression gives us a formal parametric statistical model (like linear regression with normal errors).

Our model is:

$$Y_i \sim \text{Bernoulli}(p_i), \quad p_i = F(\beta_0 + \beta_1 x_i).$$

Our model has two parameters β_0 and β_1 which can estimate given data.

We usually assume that the given the parameters and x_i, the Y_i are independent.

To estimate the parameters, we usually use *maximum likelihood*.

That is, we choose the parameter values that make the data we have seen most likely.

Let p_y be a simplified notation for $P(Y = y \mid x)$.
In the logistic model, p_y depends on (β_0, β_1)

$$p_y = p_y(\beta_0, \beta_1) = \begin{cases} P(Y = 1 \mid x) = F(\beta_0 + \beta_1 x) & Y = 1 \\ P(Y = 0 \mid x) = 1 - F(\beta_0 + \beta_1 x) & Y = 0 \end{cases}$$

For our logistic model, the probability of the $Y_i = y_i$ given x_i, $i = 1, 2, \ldots, n$ as a function of β_0 and β_1 is

$$L(\beta_0, \beta_1) = \prod_{i=1}^{n} p_{y_i}(\beta_0, \beta_1).$$

So, we estimate (β_0, β_1) by choosing the values that optimize the likelihood function $L(\beta_0, \beta_1)$!!

This optimization has to be done numerically using an iterative technique (Newton's Method!!).

The problem is convex and the optimization usually converges pretty fast.

Some fairly complex statistical theory gives us standard errors for our estimates from which we can get confidence intervals and hypothesis test for β_0 and β_1.

Here is the logistic regression output for our y=default, x= balance example.

The MLE of β_0 is $\hat{\beta}_0 = -10.65$.

The MLE of β_1 is $\hat{\beta}_1 = .0055$.

Given x=balance = 2000, $\eta = -10.65 + .0055 * 2000 = 0.35$

$\hat{\beta}_1 > 0$ suggests larger balances are associated with higher risk of default.

$P(default) = P(Y = 1 \mid x = 2000) =$ exp(.35)/(1+exp(.35)) =0.59.

```
Call:
glm(formula = default ~ balance, family = binomial, data = Default)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.2697  -0.1465  -0.0589  -0.0221   3.7589

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.065e+01  3.612e-01  -29.49   <2e-16 ***
balance      5.499e-03  2.204e-04   24.95   <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: 2920.6  on 9999  degrees of freedom
Residual deviance: 1596.5  on 9998  degrees of freedom
AIC: 1600.5

Number of Fisher Scoring iterations: 8
```

Confidence Interval for β_1:
$\hat{\beta}_1 \pm 2\text{se}(\hat{\beta}_1)$.
$.0055 \pm 2(.00022)$.

Test $H_0 : \beta_1 = \beta_1^0$
$z = \frac{\hat{\beta}_1 - \beta_1^0}{\text{se}(\hat{\beta}_1)}$.
If H_0 is true, z should look like a standard normal draw.

$\frac{.0055-0}{.00022} = 25$,
big for a standard normal
$\Rightarrow$
reject the null that $\beta_1 = 0$.

Similar for β_0.

```
Call:
glm(formula = default ~ balance, family = binomial, data = Default)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.2697  -0.1465  -0.0589  -0.0221   3.7589

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.065e+01  3.612e-01  -29.49   <2e-16 ***
balance      5.499e-03  2.204e-04   24.95   <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: 2920.6  on 9999  degrees of freedom
Residual deviance: 1596.5  on 9998  degrees of freedom
AIC: 1600.5

Number of Fisher Scoring iterations: 8
```

Fisher Scoring iterations:

It took 8 iterations of the optimization for convergence.

Deviance:

The deviance is $-2log(L(\hat{\beta}_0, \hat{\beta}_1))$.
Twice (-2) times the log of the maximized likelihood.

For numerical and theoretical reasons it turns out to be easier to work with the log of the likelihood than the likelihood itself. Taking the log turns all the products into sums.

A big likelihood is good, so a small deviance is good.

Null and Residual Deviance:

The Residual deviance is just the one you get by plugging the MLE's of β_0 and β_1 into the likelihood.

The Null deviance is what you get by setting $\beta_1 = 0$ and then optimizing the likelihood over β_0 alone.

You can see that the deviance is a lot smaller when we don't restrict β_1 to be 0!!

Deviance as a sum of losses:

If we let

$$\hat{p}_y = p_y(\hat{\beta}_0, \hat{\beta}_1),$$

then the deviance is

$$\sum_{i=1}^{n} -2 \log(\hat{p}_{y_i}).$$

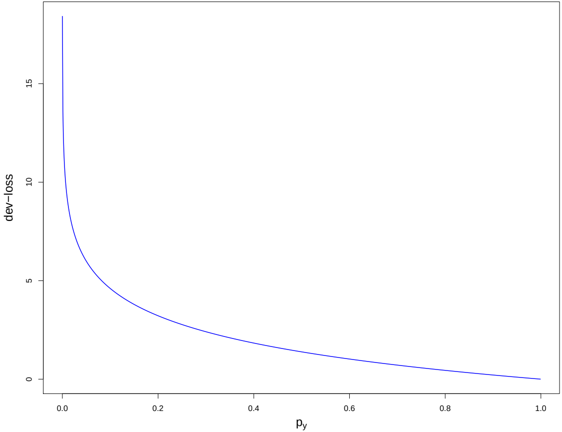
The sum over observations of -2 times the log of the estimated probability of the y you got.

p_y is the probability we assign to Y turning out to be y.
We can think of $-2\log(p_y)$ as our *loss*.

This is
p_y versus $-2\ \log(p_y)$.

When y happens, the bigger we said p_y is the better off we are, the lower our loss.

If y happens and we said p_y is small, we really get a big loss -that's fair!!



In Section 8 we will use deviance as an *out of sample* loss function, just as we have used sum of squared errors for a numeric Y.

4. Multiple Logistic Regression

We can extend our logistic model to several numeric x by letting η be a linear combination of the x's instead of just a linear function of one x:

- Step 1:
  $\eta = \beta_0 + \beta_1\, x_1 + \beta_2\, x_2 + \ldots \beta_p\, x_p.$
- Step 2:
  $P(Y = 1 \mid x = (x_1, x_2, \ldots, x_p)) = F(\eta).$

Or, in one step, our model is:

$$Y_i \sim \text{Bernoulli}(p_i), \;\; p_i = F(\beta_0 + \beta_1\, x_{i1} + \beta_2\, x_{i2} + \ldots \beta_p\, x_{ip}).$$

Our first step keeps some of the structure we are used to in linear regression.

We combine the x's together into one weighted sum that we hope will capture all the information they provide about y.

We then turn the combination into a probability by applying F.

Inference as in the $p = 1$ case discussed previously except now our likelihood will depend on $(\beta_0, \beta_1, \ldots, \beta_p)$ instead of just (β_0, β_1).

The Default Data, More than One x

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
```

Everything is analogous to when we had one x.

The estimates are MLE.

Confidence intervals are estimate +/- 2 standard errors.

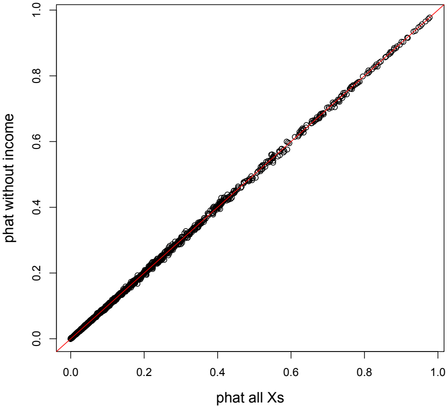
Z-stats are (estimate-proposed)/se.

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.

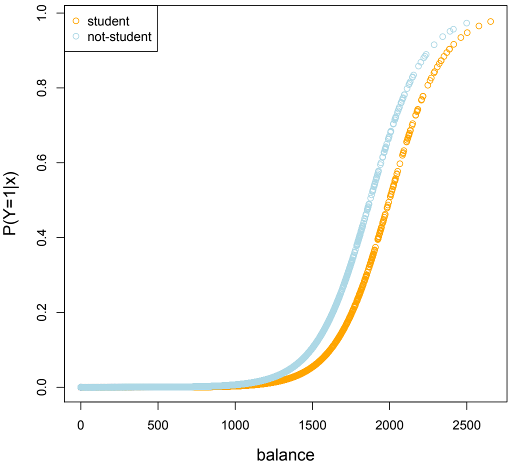
Here is the output using balance and student.

```
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
```

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.



Confounding Example:

The ISLR book notes a nice example of “confounding” in the Default data.

Suppose we do a logistic regression using only `student`.

Here the coefficient for the student dummy is positive, suggesting that a student is more likely to default.

But, in the multiple logistic regression, the coefficient for student was -.7 and we saw the a student was less likely to default at any fixed level of `balance`.

```
Call:
glm(formula = default ~ student, family = binomial, data = Default)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-0.2970  -0.2970  -0.2434  -0.2434   2.6585

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.50413    0.07071  -49.55  < 2e-16 ***
studentYes   0.40489    0.11502    3.52 0.000431 ***
---
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: 2908.7  on 9998  degrees of freedom
AIC: 2912.7

Number of Fisher Scoring iterations: 6
```

How can this be?

This is the sort of thing where our intuition from linear multiple regression can carry over to logistic regression. Since both methods start by mapping a p dimensional x down to just one number, the have some basic features in common. That is a nice thing about using logistic regression.

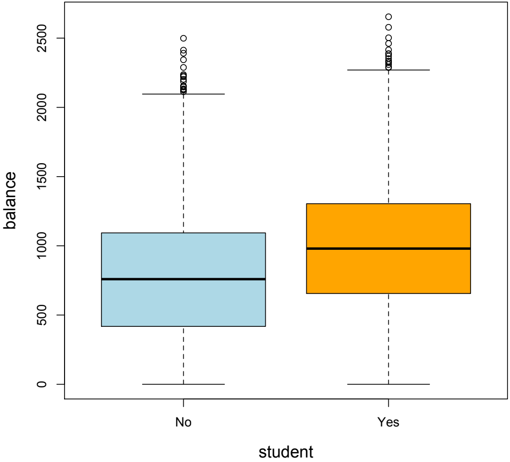
We know that when x's are correlated the coefficients for old x's can change when we add new x's to a model.

Are `balance` and `student` "correlated"?

Here is a plot of `balance` vs. `student`.
We can see the are related.

If all you know is that a credit card holder is a student, then (in the background) they are more likely to have a larger balance and hence more likely to default.

But, if you know the balance, a student is less likely to default than a non-student.



5. AIC and BIC in Logistic Regression

We have reported logistic regression results for a variety of choices for x.

- balance:
  Residual deviance: 1596.5, AIC: 1600.5
- balance + student + income:
  Residual deviance: 1571.5, AIC: 1579.5
- balance + student:
  Residual deviance: 1571.7, AIC: 1577.7
- student:
  Residual deviance: 2908.7, AIC: 2912.7

A smaller residual deviance indicates a better fit.
But, it can only get smaller when you add variables!

The deviance is just -2 times the maximized log likelihood. When you add x variables the maximized likelihood can only get bigger so the deviance can only get smaller.

If you have more coefficients to optimize over you can only do better since you can set them to zero if you want.

This is analogous to the fact that in linear multiple regression R^2 can only go up when you add x's.

AIC is analogous to the BIC and adjusted R^2 in that it penalizes you for adding variables.

Rather than choosing the model with the smallest deviance, some people advocate choosing the model with the smallest AIC value:

$$AIC = -2log(\hat{L}) + 2(p+1) = deviance + 2(p+1),$$

where $\hat{L}$ is maximized likelihood and p is the number of xs (we add 1 for the intercept).

The idea is that as you add variables (the model gets more complex), deviance goes down but 2*(p+1) goes up.

The suggestion is to pick the model with the smallest AIC.

AIC for the Default example:

A parameter (a coefficient) costs 2.

- 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).
- balance + student:
  Residual deviance: 1571.7, AIC: 1577.7 = 1571.7 + 2*(3).
- student:
  Residual deviance: 2908.7, AIC: 2912.7 = 2908.7 + 2*(2).

$\Rightarrow$ 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: $= 2908.7 + 9.2*(2) = 2927.1$.

$\Rightarrow$ 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 !!!

6. Log Odds

Logistic regression and linear regression both start with the same first key step: take a possibly high dimensional x and map it down to a single number using a linear combination of the components of x.

This reduces the dimension from p down to 1!!

Linear regression adds noise, while logistic regression just maps the single number to a probability.

$\eta_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots \beta_p x_{ip}$.

Linear Regression: $Y_i = \eta_i + \epsilon_i$.
Logistic Regression: $Y_i \sim Bernoulli(p_i), p_i = F(\eta_i)$.

Linear regression (without transformations!) is interpretable.

The non-linear F in logistic regression makes it somewhat less interpretable.

We can invert F to express our model in terms of the *odds ratio* $\frac{p}{1-p}$.

$$p = F(\eta) = \frac{e^{\eta}}{1 + e^{\eta}} \Rightarrow \log(\frac{p}{1-p}) = \eta.$$

So, we can write the logistic model as:

$$Y_i \sim Bernoulli(p_i),$$
$$\log\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots \beta_p x_{ip}.$$

Some people find this more interpretable.

7. Making Decisions

Let's consider the simple (*but very important*) case where Y is 0 or 1.

If $p(x)$ is our estimate of $P(Y = 1 \mid x)$ the obvious thing to do is classify (predict) $Y = 1$ if $p(x) > .5$. We can then look at the missclassification rate.

Sometimes we need to consider the consequences of our actions more carefully!

The simple rule "guess $Y = 1$ if $p(x) > .5$" may not be appropriate.

Target Marketing:

You are trying to decide whether or not to mail a promotion to a household.

$Y = 1$ if they buy something (when mailed the promotion)
and 0 if they don't.

x: stuff about the household

- demographics
- past purchase history.

$p(x)$:

Probability household like x, will buy when prompted by promotion.

$p(x)$: Probability household like x, will buy when prompted by promotion.

Typically, in target marketing applications, almost all $p(x)$ are less than .5!!!

It does not make sense to predict that nobody will buy and consequently send out zero promotions.

In this application, $p(x) = .1$ is *huge* since there a "real" chance they will respond and then spend an amount which is large relative to the cost of the mailing.

Minimizing Expected Loss

In our Target Marketing example you want to mail a promotion if:

- $p(x)$, the probability of a purchase is big.
- A, the average amount spent is big.
- c, the cost of a mailing is small.

Let's formally go through how you make the decision to send a mailing given these inputs.

Of course, in a given target marketing problem there may be other factors to consider, but this simple framework allows us to explore the idea of using probability to make a decision.

General Framework:

In general let's assume we are uncertain about Y,
which will be 1 or 0.

We have to decide to do something, or not: $d = 1$ means you do it, 0 means you do not.

There are then four different possible outcomes depending on the random Y and our decision.

Let $L(y, d)$ be the loss if $Y = y$ and you decide d,
where y and d are 0 or 1.

Let $L(y, d)$ be the loss if $Y = y$ and you decide d, where y and d are 0 or 1.

Make the decision which gives the smallest expected loss!

		d	
		0	1
y	0	$L(0,0)$	$L(0,1)$
	1	$L(1,0)$	$L(1,1)$

if $d = 0$, expected loss is:

$E(L(Y,0)) =$
$(1 - p(x))\, L(0,0) + p(x)\, L(1,0)$

if $d = 1$, expected loss is:

$E(L(Y,1)) =$
$(1 - p(x))\, L(0,1) + p(x)\, L(1,1)$

Our optimal decision is:

$d(x) = 1$ if:

$$(1 - p(x))\, L(0,1) + p(x)\, L(1,1) < (1 - p(x))\, L(0,0) + p(x)\, L(1,0).$$

and 0 otherwise.

Target Marketing:

		d	
		0	1
y	0	0	c
	1	A	c

if $d = 0$, expected loss is:

$p(x)\, A$

if $d = 1$, expected loss is:
c

Optimal decision:

$$d(x) = \begin{cases} 0 & p(x)\, A < c \\ \\ 1 & c < p(x)\, A \end{cases}$$

Pretty obvious: mail if expected benefits are greater than the cost.

Given our decision rule, we can express our loss in terms of Y and x:

$$L(y,x) = L(y,d(x)).$$

Target Marketing:

$$L(y,x) = L(y,d(x)) = \begin{cases} c & p(x) > \frac{c}{A} \\ \\ y\,A & p(x) < \frac{c}{A} \end{cases}$$

Clearly, the rule classify $Y = 1$ if $p(x) > .5$ is not relevant!

Another Credit Example

Assume we were after a predictive model to determine who is a good customer, i.e., who has a high probability of paying back the loan. (What tools did we use here?)

So, when a new customer walks in the bank and asks for a loan we are able to predict the probability of payback given a set of customers characteristics (features)... this could be
$\hat{p} = 0.3$, $\hat{p} = 0.5$, $\hat{p} = 0.8$...
We need to decide on a cutoff to extend or not the loan

Why not just choosing 0.5, i.e., if a costumer is more likely than not to pay, give him the money?

Another Credit Example

Well, we might have different costs associated with a default and not given a loan to a potentially good customer. In classification lingo, a **false-positive** might cost more than a **false-negative**!

For example, imagine we have the following cost table for this situation:

	Loan	No-loan
$(1-p)$	500	0
p	0	100

The expected cost under "loan" is $500(1-p)$
The expected cost under "no-loan" is $100p$

The costs are equal when $p = 5/6$... therefore we only loan money to customer with a $\hat{p} > 5/6$!

8. Out of Sample

We have seen how loss considerations help us decide on an good decision in the face of an uncertain binary Y.

A good $p(x)$ is one where our average *out of sample* loss is smallest!!

We want

$$E(L(Y, d(X))$$

to be small where the expectation E averages over future (Y, X) pairs.

Given out-of-sample observations (X_i^0, Y_i^o), $i = 1, 2, \ldots, m$ we estimate the out-of-sample expected loss with

$$\frac{1}{m}\sum_{i=1}^{m} L(Y_i^o, d(X_i^o)).$$

Note:

We do the same thing for numeric Y!!!

Our notation for numeric Y is to predict Y given $X = x$ with $d(x) = \widehat{f(x)}$.

Our loss is then

$$L(y, x) = L(y, d(x)) = (y - \widehat{f(x)})^2.$$

We estimate the out of sample expected loss with:

$$MSE^o = \frac{1}{m} \sum_{i=1}^{m} (Y_i^o - \widehat{f(X_i^o)})^2$$

We often then take the square root to put the units on the original Y scale giving $RMSE^o$.

Deviance As Out of Sample Loss

In our target marketing example, we thought about the actual consequences of our decision in our applied context to come up with our loss. *This is the right thing to do!*

Often however, we are not sure how we want to use our predictor, or are just too plain busy to think about it carefully.

In this case, a generic loss is useful.

For numeric Y MSE (or $RMSE$) are the most commonly used generic loss functions.

For classification problems with categorical Y, we often use the missclassification rate (see Section 1) for the decision rule which picks the most likely outcome.

In the binary Y case, our targeting marketing example illustrates the point that a lot of time we have important fit and $p(x) < .5$ for almost all x.

The ROC curve and the lift look at the performance of the rule $p(x) < s$ as s is varied from 0 to 1.

Alternatively, the *deviance* is used as a generic loss function for classification problems.

Deviance Loss:

Let

$$\hat{p}_y = \widehat{P(y \mid x)}.$$

Given out-of-sample observations (X_i^0, Y_i^o), $i = 1, 2, \ldots, m$ we estimate the out-of-sample expected loss with

$$\sum_{i=1}^{m} -2 \, \log(\hat{p}_{Y_i^o}).$$

As discussed in section 3, this is just the sum of our losses when Y_i^o happens and we had assigned that outcome probability $\hat{p}_{Y_i^o}$.

Default Data

Let's go back to the default data and use out of sample performance to do variable selection.

Let's do a simple train/test split.

- train: randomly pick 75%.
- test: the remaining 25%.

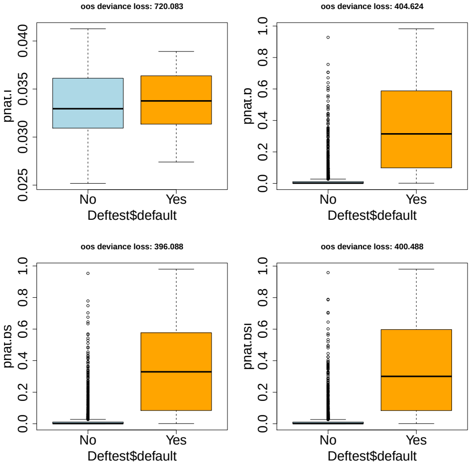
For each choice of variables, fit on train
and then plot $y = default$ vs $\widehat{p(x)}$ *for the test data*.

(1,1):
x is income.
out of sample deviance loss: 720.083.

(1,2):
x is balance.
out of sample deviance loss: 404.624.

(2,1):
x is balance+student.
out of sample deviance loss: 396.088.

(2,1):
x is balance+student+income.
out of sample deviance loss: 400.488.



Looks like just using x=balance works pretty good!!

Let's put the train/test split into a loop (like cross-validation) to make sure our result is not sensitive to our random split.

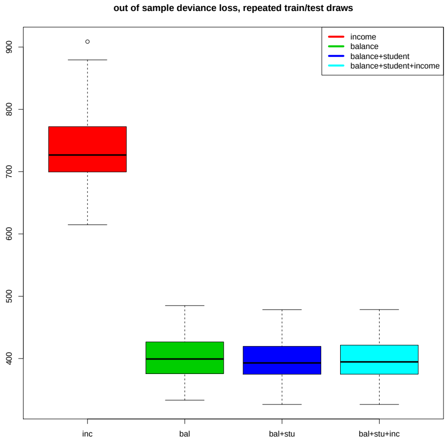
100 times we randomly split into train/test (75/25).
Each time we compute the out-of-sample deviance loss for each choice of variables.

Income alone is terrible.

No "significant" difference between the other three.

Just x=balance

still looks good!



9. Lift and ROC

Lift and ROC are two popular methods for assessing the quality of a classifier for a binary y.

Lift is particularly popular in Marketing.

ROC stands for the incomprehensible term "receiver operator characteristics".

Both look at missclassification rates for various values of s using the rule: classify $Y = 1$ if $p(x) > s$.

Let's look at our trusty default data again.

Of course, it is interesing to think about what your actual decision problem is in the default data context!!!

Kick them out if $p(x) > .2$?
Send them a nasty letter if $.1 < p(x) < .2$?

Again, lift and ROC look at the performance of "$Y = 1$ if $p(x) > s$" for a variety of s values. It is not what you would actually do, but it gives a sense of how $p(x)$ is dong.

To start with, suppose $s = .5$.

We use all the data and fit a logit using x=balance.
You could (should) of course, do this out of sample.

For each observation:
$\hat{y} = 1$ if $p(x) > .5$ and 0 otherwise.

Here is the table relating y to yhat:

y		
yhat	0	1
0	9625	233
1	42	100

This table is called the *confusion matrix*.

As the book notes, a *bewildering* number of terms have been invented to talk about this simple 2×2 table!

Counts on the diagonal are success, while the off-diagonal represent the two kinds of failures you can make.

ROC and lift summarize the situation.

```
    y
yhat     0    1
   0 9625  233
   1   42  100
```

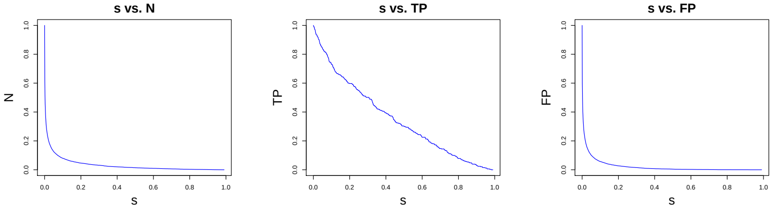
ROC looks at:

- TP (true postive), % y=1 correctly classified: $100/(100+233) = .3$.
- FP (false positive), % y=0 incorrectly classified: $42/(9625+42) = 0.0043$.

Lift looks at:

- TP (true postive), % y=1 correctly classified: .3.
- N, % classified as 1: $(100+42)/10000 = .0142$.

We then just compute these values for s between 0 and 1 and plot them.

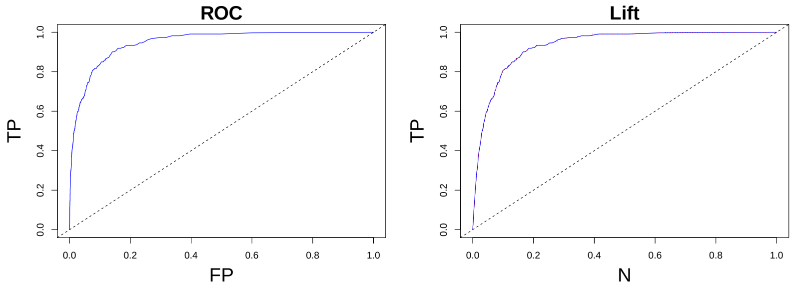


$$\hat{y} = 1 \Leftrightarrow p(x) > s.$$

- TP (true postive), % y=1 correctly classified
- FP:(false positive), % y=0 incorrectly classified
- N, % classified as 1.

All three quantities go from 1 to 0, as s goes from 0 to 1.

ROC plots FP vs. TP, and lift plots N vs. TP.



Note that as you go from left to right in these plots, s is decreasing.

The line is drawn at "y=x".
It represents the performance you would get if Y was independent of X.

More on Lift:

There is another simple way to think about the lift curve without referring to the cutoff s. Again let's using a Marketing problem to motivate things.

Suppose you have a budget that allows you to mail out to N percent of the potential customers you have on file.

For customer with information x, $p(x)$ tells you how likely they are to respond.

Given budget N, you mail out to the N percent of potential customers on file that have the large values of $p(x)$.

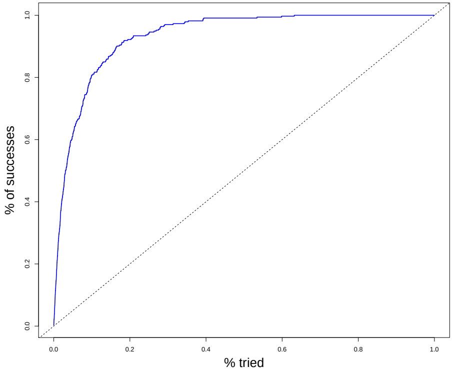
For each N (% of the ones you try) compute

$$\frac{\text{number of (y=1) from N\%}}{\text{number of (y=1) 100\%}} = \text{\% of the good ones you got.}$$

(which is just TP again).

Here is the lift again, but just relabeled:
how many you tried vs. how many of the good ones you got.

If you were just guessing, you would get $x\%$ of the good ones (on average) if you tried $x\%$ of the cases. This is captured by the straight line.



How much the lift curve is above the straight line gives you a feeling for how good $p(x)$ is.

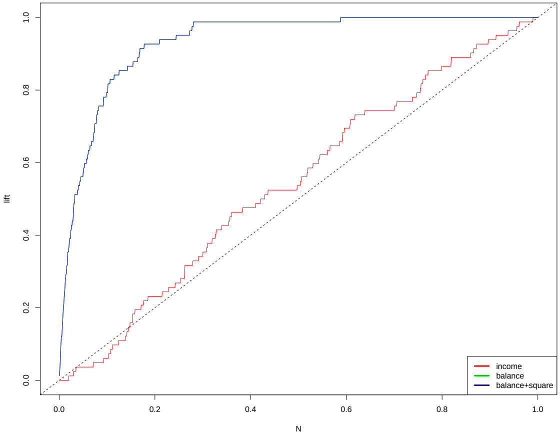
Let's use lift to compare some classifiers on the default data.

Let's try logits with:

(i) x=income.
(ii) x=balance.
(iii) x=balance + balance squared.

Each one will give us a $p(x)$ and will compare them based on their out-of-sample lift.

The lift for income is so bad, it is very close to the line.



The lift for balance + balance squared is right on top of the one for just using balance.

It did not hurt to throw in the square, but it did not help.

10. Bayes Theorem and Classification

We noted that you can think of logistic regression as a parametric model for

$$P(Y = y \mid X = x)$$

the *conditional distribution of* Y *given* $X = x$.

A number of classification techniques work by specifying the marginal distribution of Y, the conditional distribution of X given Y and then using Bayes Theorem to compute the conditional distribution of Y given X.

Conceptually, this is a very nice approach.

But it is tricky in that a lot of probability distributions have to be specified. In particular, you have to specify the possibly high-dimension distribution of X given Y.

Up to know we have been intuitive in our use of probability. Let's quickly review the basic definitions and Bayes Theorem.

10.1. Quick Basic Probability Review

Suppose X and Y are discrete random variables.

This means we can list out the possible values.

For example, suppose X can be 1,2, or 3, and Y can be 0 or 1.

Then we specify the joint distribution of (X, Y) be listing out all the possible pairs and assigning a probability to each pair:

For each possible (x, y) pair $p(x, y)$ is the probability that X turns out to be x and Y turns out to be y.

$p(x, y) = Pr(X = x, Y = y)$.

Note: X is the random variable. x is a possible value X could turn out to be.

x	y	$p(x, y)$
1	0	.894
2	0	.065
3	0	.008
1	1	.006
2	1	.014
3	1	.013

We can also arrange the probabilities in a nice two-way table.

columns:
indexed by y values

rows:
indexed by x values.

		y	
		0	1
	1	.894	.006
x	2	.065	.014
	3	.008	.013

Where did these numbers come from?

These numbers are an estimate of the joint distribution of `default` and a *discretized* version of balance from the Default data.

Y is just 1 (instead of `Yes`) for a default,
and 0 otherwise (instead of `No`).

To discretize `balance` we let X be

- 1 if balance $\leq$ 1473.
- 2 if 1473 $<$ balance $\leq$ 1857.
- 3 if 1857 $<$ balance.

This gives the simple two-way table of counts:

```
   def
bal    0    1
  1 8940   64
  2  651  136
  3   76  133
```

With corresponding percentages (divide by 10,000):

```
   def
bal     0     1
  1 0.894 0.006
  2 0.065 0.014
  3 0.008 0.013
```

Normally, we might use names like D and B for our two variables, but since we want to think about the ideas in general, let's stick with Y and X.

Joint Probabilities:

$p(x, y) = P(X = x, Y = y)$, the probability that X turns out to be x *and* Y turns out to be y is called the *joint probability*.

The complete set of joint probabilities specifies the *joint distribution* of X and Y.

Marginal Probabilities:

Give the joint distribution, we can compute the *marginal probabilities* $p(x) = P(X = x)$ or $P(Y = y)$.

$$p(x) = \sum_y p(x, y), \quad p(y) = \sum_x p(x, y).$$

Computing marginal probabilities from a joint:

P(Y=1) =
.006+.014+.013 = .033

x	y	$p(x,y)$
1	0	.894
2	0	.065
3	0	.008
1	1	.006
2	1	.014
3	1	.013

P(X=3) =
0.008+0.013 = 0.021

x	y	$p(x,y)$
1	0	.894
2	0	.065
3	0	.008
1	1	.006
2	1	.014
3	1	.013

Conditional Probabilities:

$P(Y = y \mid X = x)$ is the probability Y turns out to be y *given* you found out that X turned out to be x.

This fundamental concept is how we quantify the idea of updating our beliefs in the light of new information.

$$P(Y = y \mid X = x) = \frac{p(x,y)}{p(x)}.$$

The fraction of times you get x and y out of the times you get x.

or,

$$p(x,y) = p(x)\, p(y \mid x).$$

The chance of getting (x,y) is the fraction of times you get x times the fraction of those times you get y.

$P(Y = 1 \mid X = 3)$

$= \frac{p(3,1)}{p(3)}$

$= \frac{.013}{.008+.013}$

$= \frac{.013}{.021} = .62.$

x	y	$p(x,y)$
1	0	.894
2	0	.065
3	0	.008
1	1	.006
2	1	.014
3	**1**	**.013**

$P(X = 3 \mid Y = 1)$

$= \frac{p(3,1)}{p(1)}$

$= \frac{.013}{0.006+0.014+0.013}$

$= \frac{.013}{.033} = .394.$

x	y	$p(x,y)$
1	0	.894
2	0	.065
3	0	.008
1	1	.006
2	1	.014
3	**1**	**.013**

You just renormalize the relevant probabilities given the information!!

Compare:

P(Y=1) = .033

P(X=3) = .021.

10.2. Conditional Probability and Classification

Clearly, we can use $P(Y = y \mid X = x)$ to classify given a new value of x.

The most obvious thing to do is predict the y that has the highest probability.

Given $x = x_f$, we can predict Y to be y_f where

$$P(Y = y_f \mid X = x_f) = \max_y P(Y = y \mid X = x_f).$$

Remember, we are assuming there is just a small number of possible y so you just have to look at see which one is biggest.

For our example with `default` (Y) and discretized balance (X) our joint is

```
   def
bal     0     1
  1 0.894 0.006
  2 0.065 0.014
  3 0.008 0.013
```

If we simply divide each row by its sum we get the conditional of Y=default given X=balance.

```
   def
bal     0     1
  1 0.993 0.007
  2 0.823 0.177
  3 0.381 0.619
```

So, not surprisingly, if we use the max prob rule, you are classified (predicted) as a potential defaulter if balance=3.

Note:

If there are only two possible outcomes for Y, we are just picking the one with $P(Y = y \mid x) > .5$.

But, it is a nice feature of this way of thinking that it works pretty much the same if Y is multinomial (more than two possible outcomes) rather than just binomial (two outcomes).

Note:

Since the probabilities have to add up to one, the chance of being wrong is just

$$1 - \max_{y} P(Y = y \mid X = x_f).$$

So, in our previous example, the error probabilities are .007, .177, and .381 for x=default = 1,2,3 respectively.

10.3. Bayes Theorem

In the previous section we saw that if Y is discrete, and we have the joint distribution of (X, Y) we can "classify" y be computing $P(Y = y \mid X = x)$ for all possible y.

Note that a nice feature of this approach is that it naturally handles the case where Y can take on more than two values.

Logistic regression assumes two categories for Y.
There is a *multinomial* version of logistic regression but it is more complex.

When we use Bayes Theorem for classification we again compute $P(Y = y \mid X = x)$.

However we assume that we specify the joint distribution by specifying:

- the marginal distribution of Y.
- the conditional distribution of X given Y.

That is, we have to specify:

$$p(y) \text{ and } p(x \mid y).$$

"Bayes Theorem" simply says that if I give you $p(y)$ and $p(x \mid y)$, you can compute $p(y \mid x)$.

This is obvious since we know $p(x, y) = p(y)\, p(x \mid y)$ and if we have the joint we can compute either conditional.

To follow the notation in the book let's write k for $k = 1, 2, \ldots, K$ for the possible values of Y instead of y. We then want $P(Y = k \mid X = x)$.

Bayes Theorem:

$$P(Y = k \mid X = x) = \frac{p(x, k)}{p(x)} = \frac{p(x, k)}{\sum_{l=1}^{K} p(x, l)} = \frac{p(Y = k)p(x \mid k)}{\sum_{l=1}^{K} p(Y = l)p(x \mid l)}.$$

$$P(Y = k \mid X = x) = \frac{p(Y = k)p(x \mid k)}{\sum_{l=1}^{K} p(Y = l)p(x \mid l)}.$$

To further match up the notation that of the book, let

$$P(Y = k) = \pi_k, \text{ and } p(x \mid k) = f_k(x).$$

We then have:

$$P(Y = k \mid X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}.$$

(see equation 4.10 in the book)

Default Example:

In our example, the idea is that you start off knowing

(I) The Marginal of Y.

$$\pi_1 = P(Y = 1) = .9667, \;\; \pi_2 = P(Y = 2) = .0333.$$

(now $k = 2$, annoyingly, means a default and $k = 1$ means no default.)

(II) the conditional distribution of X for each y

```
   def
bal     1     2
  1 0.925 0.182
  2 0.067 0.424
  3 0.008 0.394
```

Take the table giving the joint $p(x, y)$ and renormalize the columns so that they add up to one.

Column 1 is $P(X = x \mid Y = 1) = f_1(x)$.
Column 2 is $P(X = x \mid Y = 2) = f_2(x)$.

So, for example,

$P(X = 2 \mid Y = 1) = f_1(2) = .067$.

So, suppose you know $X = 3$, how to you classify Y?

$$
\begin{aligned}
P(Y = 2 \mid X = 3) &= \frac{\pi_2 f_2(3)}{\pi_1 f_1(3) + \pi_2 f_2(3)} \\
&= \frac{.0333 * .394}{.9667 * .008 + .0333 * .394} \\
&= \frac{.013}{.008 + .013} \\
&= .62.
\end{aligned}
$$

as before.

Even though defaults ($Y = 2$) are unlikely, *after seeing X=3, Y=2 is likely because seeing X=3 is much more likely if Y=2 (.394) than if Y=1 (.008)*.

Note:

The π_k are called the *prior* class probabilities.
This is how likely you think $Y = k$ is *before* you see $X = x$.

Note:

A succinct way to state Bayes Theorem is

$$P(Y = k \mid X = x) \propto \pi_k \, f_k(x).$$

where $\propto$ means "proportional to".

$P(Y = k \mid X = x)$ is called the *posterior* probability that $Y = k$.

This is how likely you think $Y = k$ is *after* you see $X = x$.

$$P(Y = k \mid X = x) \propto \pi_k \, f_k(x)$$

π_k: how likely case k is for Y before you see the data x.
$f_k(x)$: how likely the data x is, given Y is in case k.

Here, $f_k(x)$ is our *likelihood*, it tells us how likely what we saw is for different values of k.

Basic Intuition: If you see something that was likely to happen if $Y = k$, maybe $Y = k$!!

$$\textit{posterior} \propto \textit{prior} \; \times \; \textit{likelihood}.$$

Bayes Theorem beautifully combines our prior information with the information in the data.

Let's redo the example using the proportional form of the formula:

$$\begin{aligned} P(Y = 1 \mid X = 3) &\propto \pi_1 f_1(3) \\ &= .9667 * .008 \\ &= 0.0077336. \end{aligned}$$

$$\begin{aligned} P(Y = 2 \mid X = 3) &\propto \pi_2 f_2(3) \\ &= .0333 * .394 \\ &= 0.0131202. \end{aligned}$$

$$P(Y = 2 \mid X = 3) = \frac{0.0131202}{0.0077336 + 0.0131202} = .629.$$

as before.

Note:

There is a lot of theory that basically says Bayes Theorem is the right thing to do.

However this assumes the π_k and $f_k(x)$ are "right", and we are almost never sure of this.

10.4. Naive Bayes

$$P(Y = k \mid X = x) \propto \pi_k \, f_k(x)$$

To make this exciting we need to make x high dimensional!!

Since we are doing classification, we still think of Y as a discrete random variable so we think of the π_k the same way.

However, now we want to think of x as possibly containing many variables.

Now X is a vector of random variables $X = (X_1, X_2, \ldots, X_p)$.

Our probability laws extend nicely in that we still have

$$p(x, y) = P(X = x, Y = y) = p(y)p(x \mid y) = p(x)p(y \mid x)$$

If each X_i is discrete,

$$p(x) = P(X = x) = P(X_1 = x_1, X_2 = x_2, \ldots, X_p = x_p).$$

and,

$$f_k(x) = P(X_1 = x_1, X_2 = x_2, \ldots, X_p = x_p \mid Y = k).$$

And we still have

$$P(Y = k \mid X = x) \propto \pi_k \, f_k(x)$$

Our problem is now obvious.

In practice, how do you specify

$$f_k(x) = P(X_1 = x_1, X_2 = x_2, \ldots, X_p = x_p \mid Y = k).$$

for large p.

This would involve understanding something about the high dimensional x.

The naive Bayes solution is to assume that, conditional on Y, all the X_i are independent.

Let's do $p = 2$ first so we can simply see what this implies.
It is always true that:

$$\begin{aligned} f_k(x) &= f_k(x_1, x_2 \mid Y = k) \\ &= P(X_1 = x_1, X_2 = x_2 \mid Y = k) \\ &= P(X_1 = x_1 \mid Y = k)\, P(X_2 = x_2, X_1 = x_1 \mid Y = k). \end{aligned}$$

Naive Bayes then assumes that

$$P(X_2 = x_2, X_1 = x_1 \mid Y = k) = P(X_2 = x_2 \mid Y = k).$$

(given Y, X_1 has no information about X_2)

So,

$$f_k(x) = f_k^1(x_1)\, f_k^2(x_2), \;\; f_k^i(x_i) = P(X_i = x_i \mid Y = k).$$

Naive Bayes:

For general p we have:

$$f_k(x) = \prod_{i=1}^{p} f_k^i(x_i)$$

and, as before,

$$P(Y = k \mid X = x) \propto \pi_k \, f_k(x)$$

Default Example:

Will will do $p = 2$ by using student status in addition to balance. Let's think of balance (still discretized) as x_1 and student status as x_2. Student status is a binary variable.

The simple part of Naive Bayes, is that we look at the components of x one at a time.

So, we still use:

```
   def
bal     1     2
  1 0.925 0.182
  2 0.067 0.424
  3 0.008 0.394
```

$$P(X_1 = 2 \mid Y = 1) = f_2^1(3) = .394.$$

.

Here is the joint of $(X_2, Y) =$ (student,default).

```
       def
student     1     2
    No  0.685 0.021
    Yes 0.282 0.013
```

Here are the conditionals of student, given $Y = 1$ or 2.

```
       def
student     1     2
    No  0.708 0.618
    Yes 0.292 0.382
```

Thinking of No and Yes as 1 or 2, we have, for example:
$f_1^2(2) = P(X_2 = 2 \mid Y = 1) = .292.$

OK, we ready to go, our information is:

(I) The Marginal of Y=default.

$$\pi_1 = P(Y = 1) = .9667, \;\; \pi_2 = P(Y = 2) = .0333.$$

(II) The conditional distributions of X_1=balance and X_2=student

```
   def
bal     1     2
  1 0.925 0.182
  2 0.067 0.424
  3 0.008 0.394
```

```
          def
student     1     2
    No  0.708 0.618
    Yes 0.292 0.382
```

So, suppose you know $X_1 = 3$ and $X_2 = 2$, how to you classify Y?

$$\begin{aligned} P(Y = 1 \mid X_1 = 3, X_2 = 2) &\propto \pi_1 f_1^1(3)\, f_1^2(2) \\ &= .9667 * .008 * .292. \\ &= 0.002258211. \end{aligned}$$

$$\begin{aligned} P(Y = 2 \mid X_1 = 3, X_2 = 2) &\propto \pi_2 f_2^1(3)\, f_2^2(2) \\ &= .0333 * .394 * .382 \\ &= 0.005011916. \end{aligned}$$

$$P(Y = 2 \mid X_1 = 3, X_2 = 2) = \frac{0.005011916}{0.002258211 + 0.005011916} = .689.$$

Note:

Just knowing $X_1 = 3$ (high balance) we got $P(Y = 2 \mid \mathit{info}) = .62$ (probability of a default is .62).

Knowing $X_1 = 3$ (high balance) *and* $X_2 = 2$ (a student) we got $P(Y = 2 \mid \mathit{info}) = .69$ (probability of a default is .69.)

Knowing the student status changed things quite a bit.

Note:

If you compare the calculation of $\pi_k \, f_k(x)$ with just X_1 versus the one with X_1 and X_2, we see that we just multiplied in an additional term for $P(X_2 = 2 \mid Y = k) = f_k^2(2)$.

With more x's you would just keep multiplying in an additional contribution for each X_j, $j = 1, 2, \ldots, p$!!!

The "scales" beautifully, in that the computation is linear in p.

But

(i)

You do have to think carefully about each X_j to come up with it's conditional given Y.

(ii)

The word "naive" in the name comes from the assumption that the X's are independent given Y.

We know balance and student are not independent, but are they independent given the default status?

However the folklore is that Naive Bayes works surprisingly well!!

Discriminant Analysis

Note:

The book discusses linear (LDA) and quadratic (QDA) discriminant analysis.

These are both example of $P(Y = k \mid X = x) \propto \pi_k \, f_k(x)$, but involve specific choices for f_k.

LDA:

$$X \mid Y = k \sim N_p(\mu_k, \Sigma).$$

QDA:

$$X \mid Y = k \sim N_p(\mu_k, \Sigma_k).$$

where $N_p(\mu, \Sigma)$ is the multivariate normal distribution.

A key observation is that the beautiful formula

$$P(Y = k \mid X = x) \propto \pi_k \, f_k(x)$$

still works when x is continuous.

When x is continuous, $f_k(x)$ is the joint density of x given $Y = k$ rather than $P(X = x \mid Y = k)$.