Logistic Regression

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Contents

1 The classification problem

We move now from the regression problem to the classification problem. The setting for the classification problem is similar to that of the regression problem. We have a response variable y and p explanatory variables $x_1, \dots, x_p$. We collect data from n subjects on these variables.

The only difference between regression and classification is that in classification, the response variable y is binary (takes only two values; for our purposes we assume it is coded as 0 and 1) while in regression, the response variable is continuous. The explanatory variables, as before, are allowed to be both continuous and discrete.

There are many examples for the classification problem. Two simple examples are given below. We shall look at more examples later on.

1.1 Frogs Dataset

This dataset is available in R via the package DAAG.

```
library(DAAG)
data(frogs)
```

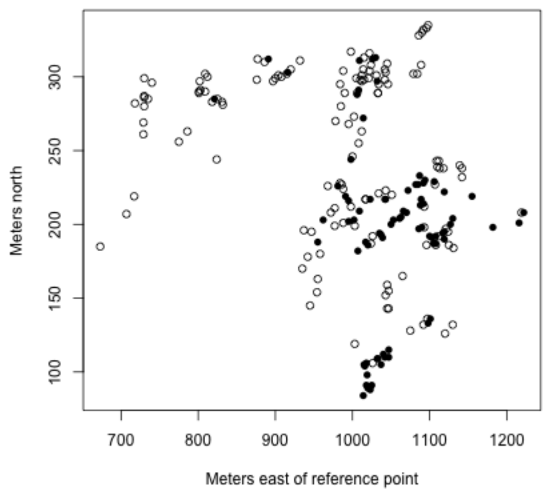
212 sites of the Snowy Mountain area of New South Wales, Australia were surveyed to understand the distribution of the Southern Corroboree frog. The variables are

1. pres.abs – 0/1 indicates whether frogs were found.
2. easting – reference point
3. northing – reference point
4. altitude – altitude in meters
5. distance – distance in meters to nearest extant population
6. NoOfPools– number of potential breeding pools
7. NoOfSites– number of potential breeding sites within a 2 km radius
8. avrain – mean rainfall for Spring period
9. meanmin – mean minimum Spring temperature

10. meanmax – mean maximum Spring temperature

The variable *easting* refers to the distance (in meters) east of a fixed reference point. Similarly *northing* refers to the distance (in meters) north of the reference point. These two variables allow us to plot the data in terms of a map as follows:

```
plot(northing ~ easting, data = frogs, pch = c(1, 16)[frogs$pres.abs +
    1], xlab = "Meters east of reference point", ylab = "Meters north")
```



In this plot, the filled points are for sites where frogs were found.

A natural goal is to under the relation between the occurance of a frog (`pres.abs`) variable and the other geographic and environmental variables. This naturally falls under the classification problem because the response variable `pres.abs` is binary.

1.2 Email Spam Dataset

This dataset is from Chapter 10 of the book *Data Analysis and Graphics* using R. The original dataset is from the UC Irvine Repository of Machine Learning. The original dataset had 4607 observations and 57 explanatory variables. The authors of the book selected 6 of the 57 variables.

```
library(DAAG)
data(spam7)
head(spam7)
```

```
##   crl.tot dollar  bang money n000 make yesno
## 1     278  0.000 0.778  0.00 0.00 0.00     y
## 2    1028  0.180 0.372  0.43 0.43 0.21     y
## 3    2259  0.184 0.276  0.06 1.16 0.06     y
## 4     191  0.000 0.137  0.00 0.00 0.00     y
## 5     191  0.000 0.135  0.00 0.00 0.00     y
## 6      54  0.000 0.000  0.00 0.00 0.00     y
```

```
spam = spam7
```

The main variable here is *yesno* which indicates if the email is spam or not. The other variables are eplanatory variables. They are:

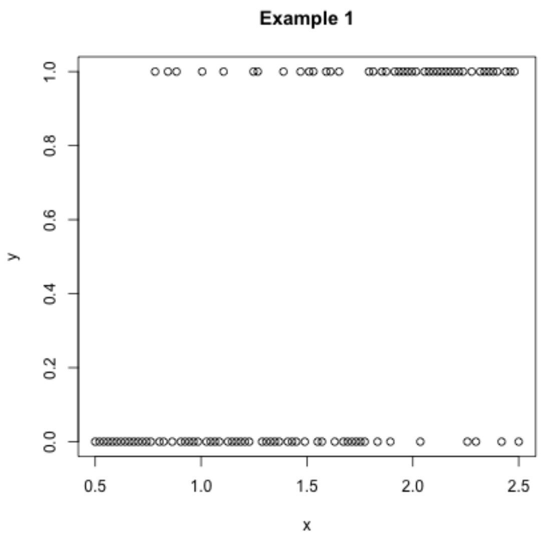
1. crl.tot - total length of words that are in capitals
2. dollar - frequency of the $ symbol, as percentage of all characters
3. bang - freqency of the symbol, as a percentage of all characters,
4. money - freqency of the word *money*, as a percentage of all words,
5. n000 - freqency of the text string *000*, as percentage of all words,
6. make - freqency of the word *make*, as a percentage of all words.

The goal is mainly to predict whether a future email is spam or not based on these explanatory variables. This is once again a classification problem because the response is binary.

There are, of course, many more examples where the classification problem arises naturally.

2 Logistic Regression Setup

We consider the simple example, where we just have a single predictor, x. We could plot our y versus our x, and might have something that looks like this (these are both toy data):



Our goal then, is to predict the value of y from our x. What do you notice about the relationship?

Logistic regression does not directly try to predict values 0 or 1, but instead tries to predict the *probability* that y is 1 as a function of its variables,

$$p(x) = P(Y = 1|x)$$

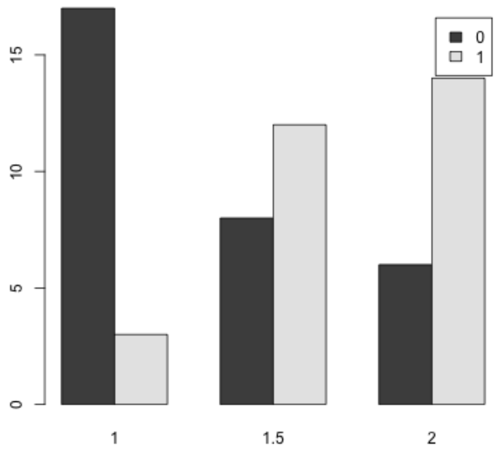
Note that this can be thought of as our model for how the data were generated: for a given value of x, you calculate the $p(x)$, and then toss a coin that has probability $p(x)$ of heads. If you get a head, $y = 1$, otherwise $y = 0$.[1]

Note that unlike regression, we are not writing y as a function of x plus noise (i.e. plus a random noise term). Instead we are writing $P(Y = 1)$ as a function of x; our randomness comes from the random coin toss we perform once we know x.

2.1 Estimating Probabilities

Let's think of a simpler example, where we observe many observations with the same value x, and their corresponding y:

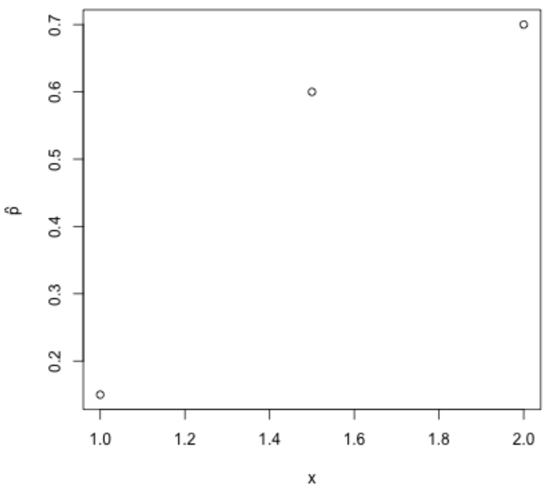
[1]I.e. conditional on x, y is distributed $Bernoulli(p(x))$.



Then how would you estimate the probability that $y = 1$ if $x = 2$?

We might then try to see how the probability of $y = 1$ is changing with x. For example, in our toy data above with the repeats above, we see a decrease in the $\hat{p}$ we estimated at each x and the probability of $y = 1$, as x increases.

```
plot(as.numeric(colnames(tab)), prop.table(tab, margin = 2)[2,
    ], xlab = "x", ylab = expression(hat(p)))
```

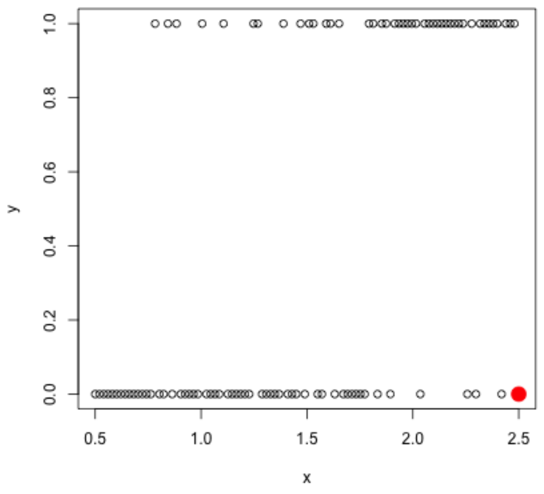


If we had this kind of data with a lot of different x values, we could think of a way to estimate how $\hat{p}(x)$ is changing with x, perhaps with curve fitting methods we've already considered.

More generally, however, we won't have multiple observations with the same x.

Without repeated observations Returning to the more realistic data, we can't do this since we only have one observation at each x value. Consider, for example, estimating the probability at $x = 2.5$ (colored in red). We only have 1 observation, and $\hat{p}(2.5) = 1$ is a *very* bad prediction based on 1 observation:

```
plot(y ~ x, data = toyDataCont)
points(y ~ x, data = subset(toyDataCont, x == 2.5),
    col = "red", pch = 19, cex = 2)
```



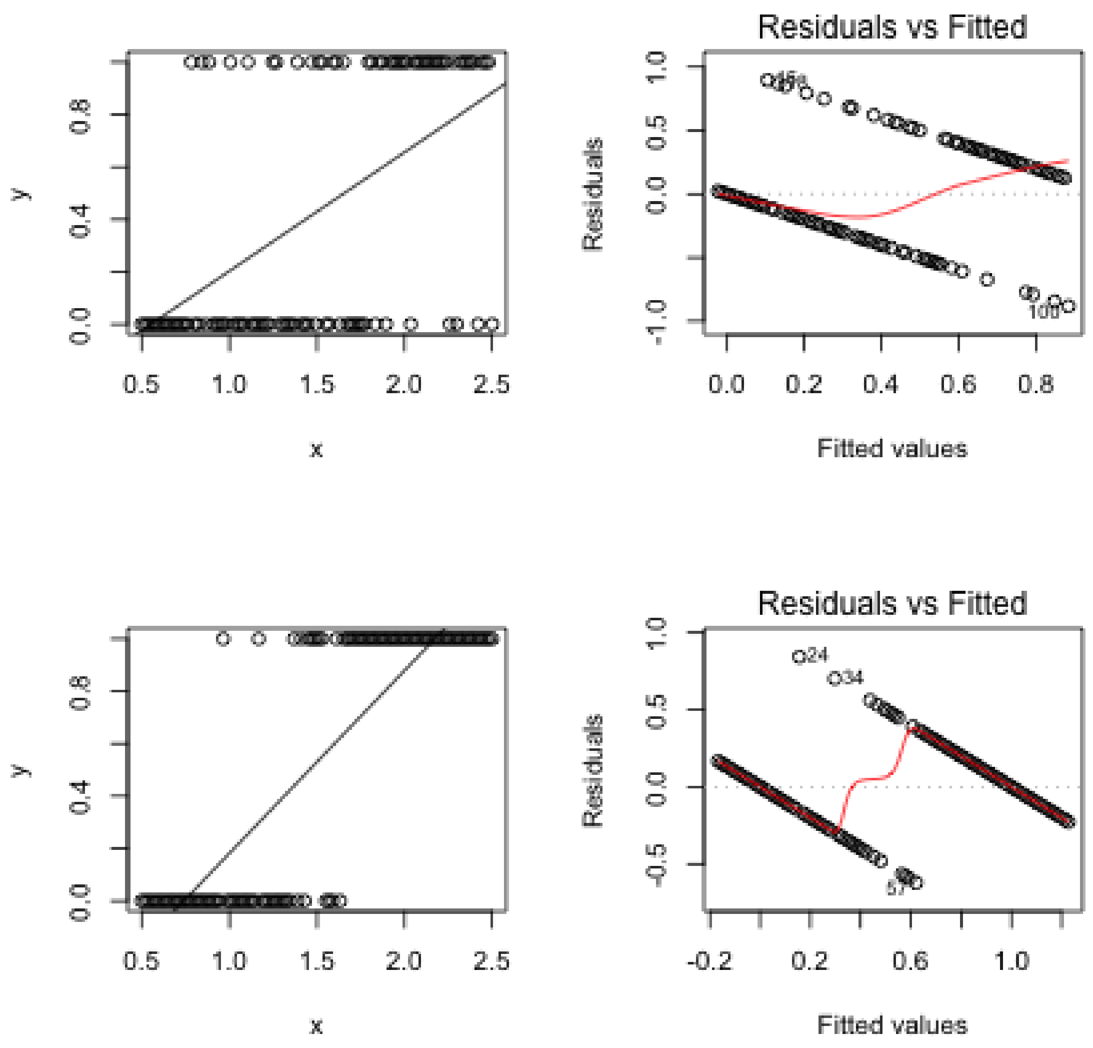
We could do something, like try to bin together similar x values, and estimate a single probability for similar values of x but creating bins gets complicated with higher dimensions (though we will see that we do something similar to this in decision trees, in the next module).

Instead, we want to predict the function $p(x)$ as some straightforward function of x.

Why not regression? We could ask, why don't we just do regression to predict $p(x)$?

Numerically, we can do it, in the sense that `lm` will give us an answer that vaguely seems reasonable. Here is the result from fitting to the toy data set above, as well as another toy data set that is similar, but with less overlap between the two classes:

```r
par(mfrow = c(2, 2))
plot(y ~ x, data = toyDataCont)
abline(lm(y ~ x, data = toyDataCont))
plot(lm(y ~ x, data = toyDataCont), which = 1)
plot(y ~ x, data = toyDataCont2)
abline(lm(y ~ x, data = toyDataCont2))
plot(lm(y ~ x, data = toyDataCont2), which = 1)
```



However, what do you notice about these predicted lines as our $\hat{p}(x)$?

This result doesn't give us a prediction for probabilities (since values are outside of [0,1]). Nor does it give us an obvious way to change our regression line into a classification (i.e. avoid predicting probabilities and just classify from the regression line); we'd have to make some decision based on our data when to decide to make a prediction of 1, and since we aren't correctly predicting probabilities, there's no obvious cutoff.

What do we do instead Instead, we want a function for $p(x)$ that is constrained within [0,1]. While we could try to figure out such a function, we are instead going to take another tack which will lead us to such a function. Specifically, we are going to consider transforming our $p(x)$ so that it takes on all real-valued values, say $z(x) = \tau(p(x))$, and then estimate $z(x)$ as a function of our x.

Why? Because now we are going to be free to use any simple modeling we've already learned to estimate $z(x)$, for example linear regression, without worrying about any constraints. Then to get $p(x)$, we will invert to get $p(x) = \tau^{-1}(z(x))$.

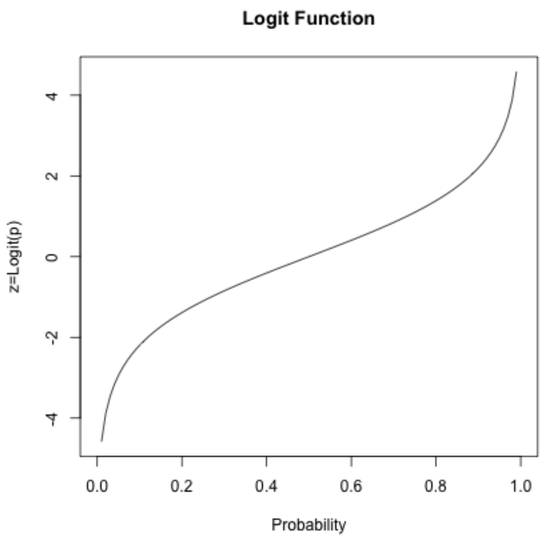
The other reason is that we are going to use a function such that $z(x) = \tau(p(x))$ actually is interpretable and makes sense on its own; thus the function $z(x)$ is actually meaningful to interpret on its own.

2.2 Logit function / Log Odds

The function we are going to use is the **logit** function,

$$z = \tau(p) = logit(p) = log(\frac{p}{1-p}).$$

```r
p <- seq(0, 1, length = 100)
z <- log(p/(1 - p))
par(mfrow = c(1, 1))
plot(p, z, type = "l", ylab = "z=Logit(p)", xlab = "Probability",
    main = "Logit Function")
```



logit(p) is interpretable as the log of the *odds*, a common measure of discussing the probability of something.

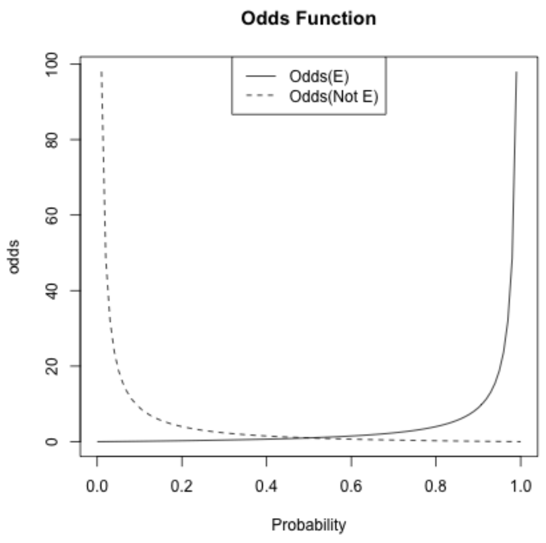
Odds If $p = P(E)$ is the probability of an event E (for example our event could be $E = y_i = 1$, and $p = P(y_i = 1)$) then the **odds** of the event E is denoted by $odds(E)$ and defined as

$$odds(E) := \frac{P(E)}{1 - P(E)} = \frac{p}{1-p} = \frac{P(E \text{ happens})}{P(E \text{ does not happen})}.$$

An important thing to note is that $P(E)$ lies between 0 and 1, while the odds ($odds(E)$) is only restricted to be nonnegative – i.e. it takes on a wider range of values. Note the following simple formulae relating probability and odds:

$$p = P(E) = \frac{odds(E)}{1 + odds(E)}$$

```r
p <- seq(0, 1, length = 100)
odds <- p/(1 - p)
par(mfrow = c(1, 1))
plot(p, odds, type = "l", ylab = "odds", xlab = "Probability",
    main = "Odds Function")
lines(p, 1/odds, type = "l", ylab = "odds", xlab = "Probability",
    main = "Odds Function", lty = 2)
legend("top", legend = c("Odds(E)", "Odds(Not E)"),
    lty = c(1, 2))
```



Log Odds From a modeling perspective, it is still akward to work with odds, for example to try to predict the odds, because it must be positive. Moreover, it's not symmetric in our choice of whether we consider $P(y = 1)$ versus $P(y = 0)$ – changes of probability of $P(y = 1)$ from 0.8 to 0.9 create large differences in the odds, but but small differences in changing from the probability from 0.2 to 0.1. This is unfortunate, since the choice of trying to estimate $P(y = 1)$ is arbitrary – we could have just as easily considered $P(y = 0)$ and modelled that.

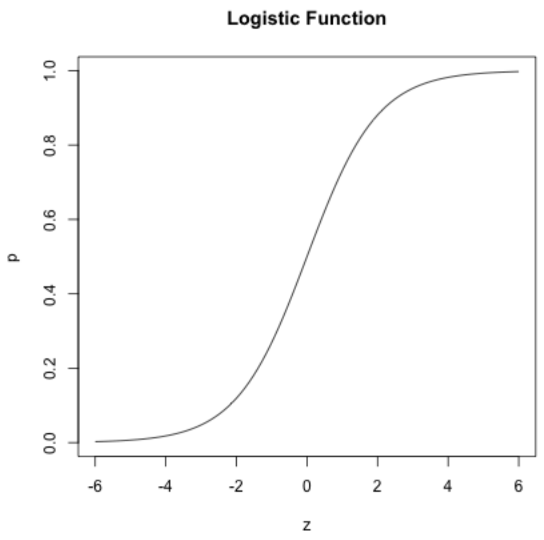
However, if we take the log of the odds, there is no restriction on $\log(odds(E))$ i.e., log-odds can take on all real-valued numbers. Moreover, the function is symmetric around 0.5, meaning that the difference between the log-odds of $p = 0.8$ versus $p = 0.9$ is the same difference as the log-odds of $p = 0.2$ versus $p = 0.1$ (see the figure above).

Converting from log-odds to probability We have the simple relationship between z, the log-odds, and the probability, $p = P(E)$

$$p = P(E) = \tau^{-1}(z) = \frac{e^z}{1 + e^z} = \frac{1}{1 + e^{-z}}.$$

This function is called the **logistic function**. For any real-valued z, the logistic function converts that number into a value between 0-1 (i.e. a probability).

```r
x <- seq(-6, 6, length = 100)
p <- exp(x)/(1 + exp(x))
par(mfrow = c(1, 1))
plot(x, p, type = "l", xlab = "z", ylab = "p", main = "Logistic Function")
```



2.3 Logistic Regression Model

Logistic regression, then, is to model the $logit(p)$ (i.e. the log-odds of the event), as a linear function of the explanatory variable values x_i of the i^{th} individual. Again, this is a feasible thing to do, since $\log odds$ take on the full range of values, so that we won't have to figure out how to make sure we don't predict probabilities outside of 0-1. Then, because of the relationships above, this gives us a model for the probabilities with respect to our explanatory variables x.

The logistic regression model, for $p = P(y = 1)$, is given as:

$$\log(\frac{p}{1-p}) = \log\left(odds(y=1)\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p.$$

This means that we are modeling the probabilities as

$$p(x) = \frac{\exp(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p)}{1 + \exp(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p)}$$

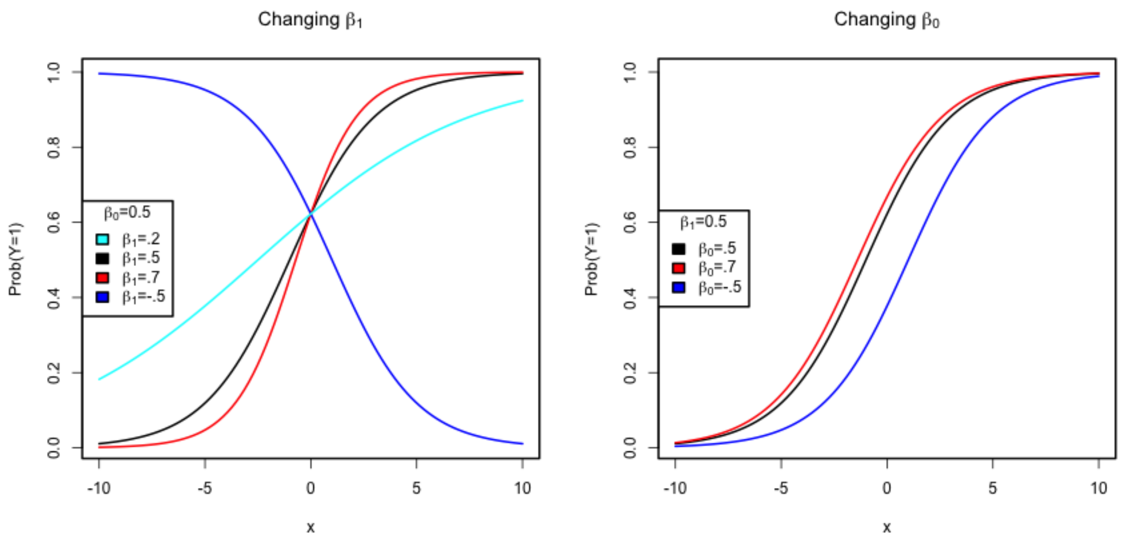
Visualizing Logistic Model To understand the effect of these variables, let's consider our model for a single variable x:

$$log(\frac{p_i}{1-p_i}) = \log(odds(y_i = 1)) = \beta_0 + \beta_1 x_i$$

which means

$$p_i = \frac{\exp\left(\beta_0 + \beta_1 x_i\right)}{1 + exp(\beta_0 + \beta_1 x_i)}$$

We can visualize the relationship of the probability p of getting $y = 1$ as a function of x, for different values of β



Fitting the Logistic Model in R The R function for logistic regression in R is *glm()* and it is not very different from *lm()* in terms of syntax.

For the frogs dataset, we will try to fit a model (but without the geographical variables)

```
frogsNoGeo <- frogs[, -c(2, 3)]
glmFrogs = glm(pres.abs ~ ., family = binomial, data = frogsNoGeo)
summary(glmFrogs)
```

```
##
## Call:
## glm(formula = pres.abs ~ ., family = binomial, data = frogsNoGeo)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.7215  -0.7590  -0.2237   0.8320   2.6789
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept)  1.105e+02  1.388e+02   0.796  0.42587
## altitude    -3.086e-02  4.076e-02  -0.757  0.44901
## distance    -4.800e-04  2.055e-04  -2.336  0.01949 *
## NoOfPools    2.986e-02  9.276e-03   3.219  0.00129 **
## NoOfSites    4.364e-02  1.061e-01   0.411  0.68077
## avrain      -1.140e-02  5.995e-02  -0.190  0.84920
## meanmin      4.899e+00  1.564e+00   3.133  0.00173 **
## meanmax     -5.660e+00  5.049e+00  -1.121  0.26224
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 279.99  on 211  degrees of freedom
## Residual deviance: 198.74  on 204  degrees of freedom
## AIC: 214.74
##
## Number of Fisher Scoring iterations: 6
```

glm stands for **generalized linear model**. Logistic regression is a special case of a generalized linear model; the *family = binomial* clause in the function tells R to fit a logistic regression equation to the data – namely what kind of function to use to determine whether the predicted probabilities fit our data.

3 Interpreting the Results

3.1 Coefficients

The parameter β_j is interpreted as the change in *log-odds* of the event $y = 1$ for a unit change in the variable x_j provided all other explanatory variables are kept unchanged. Equivalently, e^{β_j} can be interpreted as the multiplicative change in *odds* due to a unit change in the variable x_j – provided all other explanatory variables are kept unchanged.

The R function provides estimates of the parameters $\beta_0, \dots, \beta_p$. For example, in the frogs dataset, the estimated coefficient of the variable `NoOfPools` is 0.02986. This is interpreted as the change in log-odds of the event of finding a frog when the `NoOfPools` increases by one (provided the other variables remain unchanged). Equivalently, the odds of finding a frog get multiplied by $\exp(0.02986) = 1.03031$ when the `NoOfPools` increases by one.

P-values are also provided for each $\hat{\beta}_j$; they have a similar interpretation as in linear regression, namely evaluating the null hypothesis that $\beta_j = 0$. We are not going to go into how these p-values are calculated. Basically, if the model is true, $\hat{\beta}_j$ will be approximately normally distributed, with that approximation being better for larger sample size. Logistic regression significance statements rely much more heavily on asymptotics (i.e. having large sample sizes), *even if the data exactly follows the data generation model!*

3.2 Fitted Values and prediction

Now suppose a new site is found in the area for which the explanatory variable values are: altitude 1700 m, distance 400 m, NoOfPools 30, NoOfSites 8, avrain 150 (mm ??), meanmin 4 (degrees celsius ??) and meanmax is 16 (degrees celsius ??). What can our logistic regression equation say about the presence or absence of frogs in this area? Our logistic regression allows us to calculate the $\log(odds)$ of finding frogs in this area as:

```
x0 = c(1, 1700, 400, 30, 8, 150, 4, 16)
sum(x0 * glmFrogs$coefficients)
```

```
## [1] -13.58643
```

Remember that this is $\log(odds)$. From here, the odds of finding frogs is calculated as

```
exp(sum(x0 * glmFrogs$coefficients))
```

```
## [1] 1.257443e-06
```

These are very low odds. If one wants to obtain an estimate of the **probability** of finding frogs at this new location, we can use the formula above to get:

```
exp(sum(x0 * glmFrogs$coefficients))/(1 + exp(sum(x0 *
    glmFrogs$coefficients)))
```

```
## [1] 1.257441e-06
```

Therefore, we will predict that this species of frog will not be present at this new location.

Similar to fitted values in linear regression, we can obtain fitted probabilities in logistic regression for each of the observations in our sample using the `fitted` function:

```
head(fitted(glmFrogs))
```

```
##         2         3         4         5         6         7
## 0.9994421 0.9391188 0.8683363 0.7443973 0.9427198 0.7107780
```

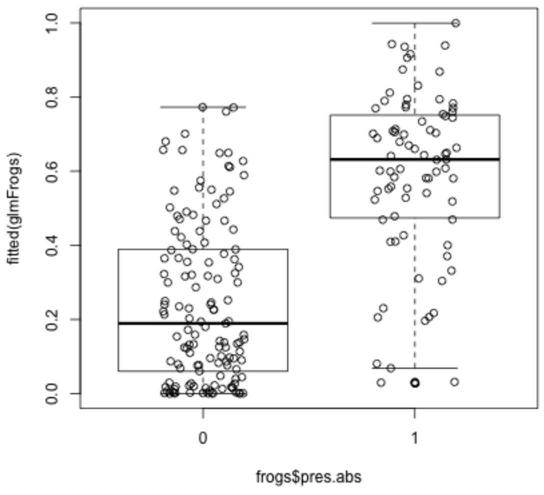
These fitted values are the *fitted probabilities* for each observation in our sample. For example, for $i = 45$, we can also calculate the fitted value manually as:

```
i = 45
rrg = c(1, frogs$altitude[i], frogs$distance[i], frogs$NoOfPools[i],
    frogs$NoOfSites[i], frogs$avrain[i], frogs$meanmin[i],
    frogs$meanmax[i])
eta = sum(rrg * glmFrogs$coefficients)
prr = exp(eta)/(1 + exp(eta))
c(manual = prr, FittedFunction = unname(glmFrogs$fitted.values[i]))
```

```
##         manual FittedFunction
##      0.5807378      0.5807378
```

The following plots the fitted values against the actual response:

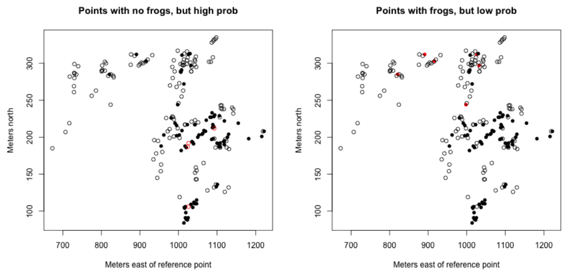
```
boxplot(fitted(glmFrogs) ~ frogs$pres.abs, at = c(0,
    1))
points(x = jitter(frogs$pres.abs), fitted(glmFrogs))
```



Why do I plot this as a boxplot?

Some of the regions where frogs were present seems to have received very low fitted probability under the model (and conversely, some of the regions with high fitted probability did not actually have any frogs). We can look at these unusual points in the following plot:

```
sel <- frogs$pres.abs == 0 & glmFrogs$fitted > 0.7
par(mfrow = c(1, 2))
plot(northing ~ easting, data = frogs, pch = c(1, 16)[frogs$pres.abs +
    1], col = c("black", "red")[factor(sel)], xlab = "Meters east of reference point"
    ylab = "Meters north", main = "Points with no frogs, but high prob")
sel <- frogs$pres.abs == 1 & glmFrogs$fitted < 0.2
plot(northing ~ easting, data = frogs, pch = c(1, 16)[frogs$pres.abs +
    1], col = c("black", "red")[factor(sel)], xlab = "Meters east of reference point"
    ylab = "Meters north", main = "Points with frogs, but low prob")
```



What do you notice about these points?

3.3 Fitting the model & Residual Deviance

We haven't discussed how we find the "best" choice of coefficients β for our model. Like regression, we are going to choose the coefficients based on getting the best fit to our data.

In regression we considered the squared residual as a measure of our fit to an observation,

$$(y_i - \hat{y}_i)^2,$$

and minimizing the average fit to our data. We will do something similar in logistic regression, but

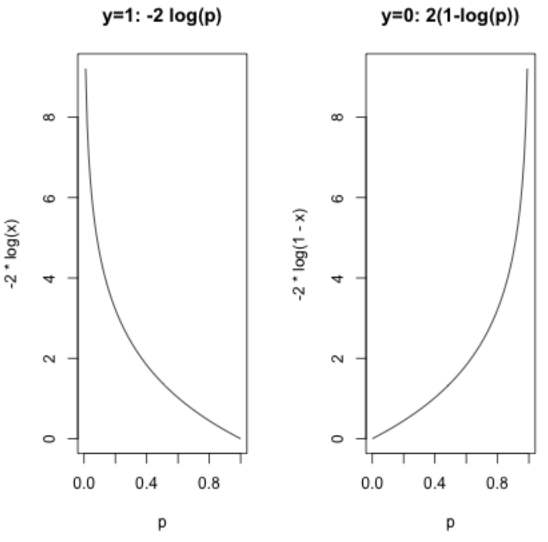
1. We will consider the fit of the fitted *probabilities*
2. the criterion we use to determine the best coefficients β is not the residual, but another notion of "fit" to every observation.

Let $\hat{p}_1, \dots, \hat{p}_n$ denote the fitted probabilities in logistic regression for a specific coefficient. The actual response values are $y_1, \dots, y_n$ (note that these are binary). If the fit is good, we would expect $\hat{p}_i$ to be small (close to zero) when y_i is 0 and $\hat{p}_i$ to be large (close to one) when y_i is 1. Conversely, if the fit is not good, we would expect $\hat{p}_i$ to be large for some y_i that is zero and $\hat{p}_i$ to be small for some y_i that is 1. A commonly used function for measuring if a probability p is close to 0 is $-2\log p$. This quantity $-2\log p$ is always nonnegative and it becomes very large if p is close to zero. Similarly, one can measure if a probability p is close to 1 by $-2\log(1-p)$. Using these quantities, we measure the quality of fit of $\hat{p}_i$ to y_i by

$$Dev(\hat{p}_i, y_i) = \begin{cases} -2\log \hat{p}_i & : y_i = 1 \\ -2\log(1-\hat{p}_i) & : y_i = 0 \end{cases}$$

This is called the **deviance**.[2]If $Dev(\hat{p}_i, y_i)$ is large, it means that $\hat{p}_i$ is **not** a good fit for y_i.

[2]This comes from assuming that the y_i follow a Bernoulli distribtion with probability p_i. Then this is the negative log-likelihood of the observation, and by minimizing the average of this over all observations, we are maximizing the likelihood.



Because y_i is either 0 or 1, the above formula for $Dev(\hat{p}_i, y_i)$ can be written more succinctly as

$$Dev(\hat{p}_i, y_i) = y_i\left(-2\log\hat{p}_i\right) + (1 - y_i)\left(-2\log(1-\hat{p}_i)\right).$$

Note that this is for the i^{th} observation. We can get a measure of the overall goodness of fit (across all observations) by simply summing this quantity over $i = 1, \ldots, n$. The resulting quantity is called the **Residual Deviance**:

$$RD = \sum_{i=1}^{n} Dev(\hat{p}_i, y_i).$$

Just like RSS, small values of RD are preferred and large values indicate lack of fit.

This doesn't have our β_j anywhere, so how does this help in choosing the best β? Well, our model says that $\hat{p}_i$ is a specific function of our x_i values:

$$\hat{p}_i = \hat{p}(x_i) = \tau^{-1}(\hat{\beta}_0 + \ldots + \hat{\beta}_p x_i^{(p)}) = \frac{\exp(\hat{\beta}_0 + \ldots + \hat{\beta}_p x_i^{(p)})}{1 + \exp(\hat{\beta}_0 + \ldots + \hat{\beta}_p x_i^{(p)})}$$

So we can put those values into our equation above, and find the $\hat{\beta}_j$ that maximize that quantity. Unlike linear regression, this *has* to be maximized by a computer – you can't write down an expression for the $\hat{\beta}_j$ that maximize this quantity equation.

Residual Deviance in R The function `deviance` can be used in R to calculate deviance. It can, of course, also be calculated manually using the fitted probabilities.

RD (Residual Deviance) can be calculated from our `glm` object as

```
deviance(glmFrogs)
```

```
## [1] 198.7384
```

4 Comparing Models

4.1 Deviance and submodels

Residual Deviances has parallels to RSS in linear regression, and we can use deviance to compare models similarly to linear regression.

RD decreases as you add variables Just like the RSS in linear regression, the RD in logistic regression will always decrease as more variables are added to the model. For example, in the frogs dataset, if we remove the variable `NoOfPools`, the RD changes to:

```
m2 = glm(pres.abs ~ altitude + distance + NoOfSites +
    avrain + meanmin + meanmax, family = binomial,
    data = frogs)
deviance(m2)
```

```
## [1] 210.8392
```

```
deviance(glmFrogs)
```

```
## [1] 198.7384
```

Note that RD decreased from 210.84 to 198.7384 by adding `NoOfPools`.

The Null Model (No Variables) We can similarly ask whether we need *any* of the variables (like the F test). The Null Deviance (ND) is the analogue of TSS (Total Sum of Squares) in linear regression. It simply refers to the deviance when there are no explanatory variables i.e., when one does logistic regression with only the intercept.

We can fit a model in R with no variables with the following syntax:

```
m0 <- glm(pres.abs ~ 1, family = binomial, data = frogs)
deviance(m0)
```

```
## [1] 279.987
```

Note, when there are no explanatory variables, the fitted probabilities are all equal to $\bar{y}$:

```
head(fitted(m0))
```

```
##         2         3         4         5         6         7
## 0.3726415 0.3726415 0.3726415 0.3726415 0.3726415 0.3726415
```

```
mean(frogs$pres.abs)
```

```
## [1] 0.3726415
```

Notice that this null deviance is reported in the summary of the full model we fit:

```
summary(glmFrogs)
```

```
##
## Call:
## glm(formula = pres.abs ~ ., family = binomial, data = frogsNoGeo)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.7215  -0.7590  -0.2237   0.8320   2.6789
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept)  1.105e+02  1.388e+02   0.796  0.42587
## altitude    -3.086e-02  4.076e-02  -0.757  0.44901
## distance    -4.800e-04  2.055e-04  -2.336  0.01949 *
## NoOfPools    2.986e-02  9.276e-03   3.219  0.00129 **
## NoOfSites    4.364e-02  1.061e-01   0.411  0.68077
## avrain      -1.140e-02  5.995e-02  -0.190  0.84920
## meanmin      4.899e+00  1.564e+00   3.133  0.00173 **
## meanmax     -5.660e+00  5.049e+00  -1.121  0.26224
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 279.99  on 211  degrees of freedom
## Residual deviance: 198.74  on 204  degrees of freedom
## AIC: 214.74
##
## Number of Fisher Scoring iterations: 6
```

Significance of submodels The deviances come with degrees of freedom. The degrees of freedom of RD is $n-p-1$ (exactly equal to the residual degrees of freedom in linear regression) while the degrees of freedom of ND is $n-1$.

Unlike regression, the automatic summary does not give a p-value as to whether this is a significant change in deviance. Similarly, the `anova` function for comparing submodels doesn't give a significance for comparing a submodel to the larger model

```
anova(m0, glmFrogs)
```

```
## Analysis of Deviance Table
##
## Model 1: pres.abs ~ 1
## Model 2: pres.abs ~ altitude + distance + NoOfPools + NoOfSites + avrain +
##     meanmin + meanmax
##   Resid. Df Resid. Dev Df Deviance
## 1       211     279.99
## 2       204     198.74  7   81.249
```

The reason for this that because for logistic regression, unlike linear regression, there are multiple tests that for the same test. Furthermore, the `glm` function can fit other models than just the logistic model, and depending on those models, you will want different tests. I can specify a test, and get back a significance value:

```
anova(m0, glmFrogs, test = "LRT")
```

```
## Analysis of Deviance Table
##
## Model 1: pres.abs ~ 1
## Model 2: pres.abs ~ altitude + distance + NoOfPools + NoOfSites + avrain +
##     meanmin + meanmax
##   Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
## 1       211     279.99
## 2       204     198.74  7   81.249 7.662e-15 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

What are the conclusions of these tests?

Comparison with Tests of $\hat{\beta}_j$ Notice that unlike linear regression, you get slightly different answers testing the importance of leaving out `NoOfPools` using the anova above and test statistics that come with the summary of the logistic object:

```
anova(m2, glmFrogs, test = "LRT")
```

```
## Analysis of Deviance Table
##
## Model 1: pres.abs ~ altitude + distance + NoOfSites + avrain + meanmin +
##     meanmax
## Model 2: pres.abs ~ altitude + distance + NoOfPools + NoOfSites + avrain +
##     meanmin + meanmax
##   Resid. Df Resid. Dev Df Deviance Pr(>Chi)
## 1       205     210.84
## 2       204     198.74  1   12.101 0.000504 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
cat("Summary results:\n")
```

```
## Summary results:
```

```
round(summary(glmFrogs)$coeff, 4)
```

```
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) 110.4935   138.7622  0.7963   0.4259
## altitude     -0.0309     0.0408 -0.7571   0.4490
## distance     -0.0005     0.0002 -2.3360   0.0195
## NoOfPools     0.0299     0.0093  3.2192   0.0013
## NoOfSites     0.0436     0.1061  0.4114   0.6808
## avrain       -0.0114     0.0599 -0.1901   0.8492
## meanmin       4.8991     1.5637  3.1329   0.0017
## meanmax      -5.6603     5.0488 -1.1211   0.2622
```

They are still testing the same null hypothesis, but they are making different choices about the statistic to use[3]; in linear regression the different choices converge to the same test (the F-statistic for ANOVA is the square of the t-statistic), but this is a special property of normal distribution. Theoretically these two choices are equivalent for large enough sample size; in practice they can differ.

4.2 Variable Selection using AIC

Although the Residual Deviance (RD) measures goodness of fit, it cannot be used for variable selection because the full model will have the smallest RD. The AIC however can be used as a goodness of fit criterion (this involves selecting the model with the smallest AIC).

AIC We can similarly calculate the AIC , only now it is based on the residual deviance,

$$AIC = RD + 2\,(p+1)$$

```
AIC(glmFrogs)
```

```
## [1] 214.7384
```

```
glmFrogs$deviance + 2 * (7 + 1)
```

```
## [1] 214.7384
```

[3]The glm summary gives the Wald-statistics, while the anova uses the likelihood ratio statistic.

Based on AIC, we have the same choices as in linear regression. In principle, one can go over all possible submodels and select the model with the smallest value of AIC. But this involves going over 2^p models which might be computationally difficult if p is moderate or large. A useful alternative is to use stepwise methods, only now comparing the change in RD rather than RSS; we can use the same `step` function in R:

```
step(glmFrogs, direction = "both", trace = 0)
```

```
##
## Call:  glm(formula = pres.abs ~ distance + NoOfPools + meanmin + meanmax,
##     family = binomial, data = frogsNoGeo)
##
## Coefficients:
## (Intercept)     distance    NoOfPools      meanmin      meanmax
##  14.0074032   -0.0005138    0.0285643    5.6230647   -2.3717579
##
## Degrees of Freedom: 211 Total (i.e. Null);  207 Residual
## Null Deviance:     280
## Residual Deviance: 199.6  AIC: 209.6
```

5 Classification Using Logistic Regression

Suppose that, for a new site, our logistic regression model predicts that the probability that a frog will be found at that site to be $\hat{p}(x)$. What if we want to make a binary prediction, rather than just a probability, i.e. prediction $\hat{y}$ that is a 1 or 0, prediction whether there will be frogs found at that site. How large should $\hat{p}(x)$ be so that we predict that frogs will be found at that site? 0.5 sounds like a fair threshold but would 0.6 be better?

Let us now introduce the idea of a **confusion matrix**. Given any chosen threshold, we can form obtain predictions in terms of 0 and 1 for each of the sample observations by applying the threshold to the fitted probabilities given by logistic regression. The confusion matrix is created by comparing these predictions with the actual observed responses.

	$\hat{y} = 0$	$\hat{y} = 1$
$y = 0$	C_0	W_1
$y = 1$	W_0	C_1

- C_0 denotes the number of observations where we were correct in predicting 0: both the observed response as well as our prediction are equal to zero.
- W_1 denotes the number of observations where were wrong in our predictions of 1: the observed response equals 0 but our prediction equals 1.
- W_0 denotes the number of observations where were wrong in our predictions of 0: the observed response equals 1 but our prediction equals 0.
- C_1 denotes the number of observations where we were correct in predicting 0: both the observed response as well as our prediction are equal to 1.

For example, for the frogs data, if we choose the threshold 0.5, then the entries of the confusion matrix can be calculated as:

```
cat("Confusion for threshold 0.5:\n")
```

```
## Confusion for threshold 0.5:
```

```
confusion(frogs$pres.abs, glmFrogs$fitted.values, 0.5)
```

```
##      C0 W1 W0 C1
## 0.5 112 21 21 58
```

On the other hand, if we use a threshold of 0.3, the numbers will be:

```
cat("Confusion for threshold 0.3:\n")
```

```
## Confusion for threshold 0.3:
```

```
confusion(frogs$pres.abs, glmFrogs$fitted.values, 0.3)
```

```
##     C0 W1 W0 C1
## 0.3 84 49 10 69
```

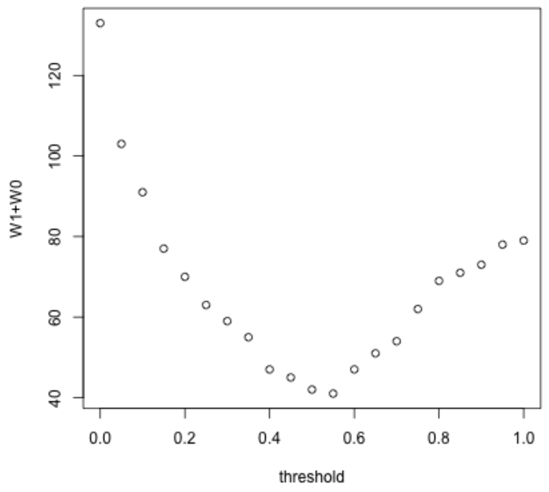
Note that C_0 and C_1 denote the extent to which the response agrees with our threshold. And W_1 and W_0 measure the extent to which they disagree. An optimal threshold can be chosen to be one which minimizes $W_1 + W_0$. We can compute the entries of the confusion matrix for a range of possible thresholds.

```
##        C0  W1 W0 C1
## 0       0 133  0 79
## 0.05   33 100  3 76
## 0.1    47  86  5 74
## 0.15   61  72  5 74
## 0.2    69  64  6 73
## 0.25   80  53 10 69
## 0.3    84  49 10 69
## 0.35   91  42 13 66
## 0.4   100  33 14 65
## 0.45  106  27 18 61
## 0.5   112  21 21 58
## 0.55  118  15 26 53
## 0.6   121  12 35 44
## 0.65  126   7 44 35
## 0.7   129   4 50 29
## 0.75  130   3 59 20
## 0.8   133   0 69 10
## 0.85  133   0 71  8
## 0.9   133   0 73  6
## 0.95  133   0 78  1
## 1     133   0 79  0
```

Notice that I can get either W_1 *or* W_0 exactly equal to 0 (i.e no mis-classifications). Why is that not a good idea?

We can then plot the value of $W_1 + W_0$ for each value of the threshold in the following plot:

```
plot(thr, conf[, "W1"] + conf[, "W0"], xlab = "threshold",
    ylab = "W1+W0")
```



The smallest value of $W_1 + W_0$ corresponds to the threshold 0.55. It is sensible therefore to use this threshold for predictions.

5.1 Example of Spam Dataset

Let us now consider the email spam dataset. Recall the dataset:

```
head(spam7)
```

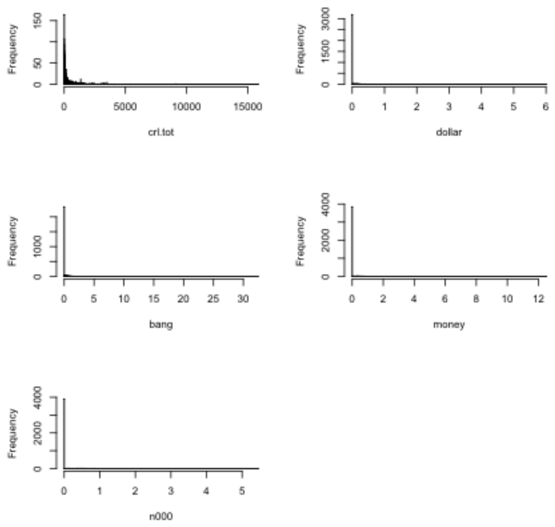
```
##   crl.tot dollar  bang money n000 make yesno
## 1     278  0.000 0.778  0.00 0.00 0.00     y
## 2    1028  0.180 0.372  0.43 0.43 0.21     y
## 3    2259  0.184 0.276  0.06 1.16 0.06     y
## 4     191  0.000 0.137  0.00 0.00 0.00     y
## 5     191  0.000 0.135  0.00 0.00 0.00     y
## 6      54  0.000 0.000  0.00 0.00 0.00     y
```

Before fitting a logistic regression model, let us first look at the summary and histograms of the explanatory variables:

```
summary(spam)
```

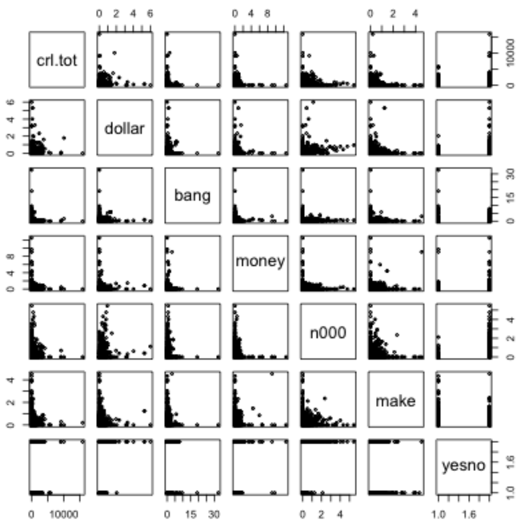
```
##     crl.tot            dollar              bang              money
##  Min.   :    1.0   Min.   :0.00000   Min.   : 0.0000   Min.   : 0.00000
##  1st Qu.:   35.0   1st Qu.:0.00000   1st Qu.: 0.0000   1st Qu.: 0.00000
##  Median :   95.0   Median :0.00000   Median : 0.0000   Median : 0.00000
##  Mean   :  283.3   Mean   :0.07581   Mean   : 0.2691   Mean   : 0.09427
##  3rd Qu.:  266.0   3rd Qu.:0.05200   3rd Qu.: 0.3150   3rd Qu.: 0.00000
##  Max.   :15841.0   Max.   :6.00300   Max.   :32.4780   Max.   :12.50000
##       n000              make         yesno
##  Min.   :0.0000   Min.   :0.0000   n:2788
##  1st Qu.:0.0000   1st Qu.:0.0000   y:1813
##  Median :0.0000   Median :0.0000
##  Mean   :0.1016   Mean   :0.1046
##  3rd Qu.:0.0000   3rd Qu.:0.0000
##  Max.   :5.4500   Max.   :4.5400
```

```
par(mfrow = c(3, 2))
for (i in 1:5) hist(spam[, i], main = "", xlab = names(spam)[i],
    breaks = 10000)
par(mfrow = c(1, 1))
```



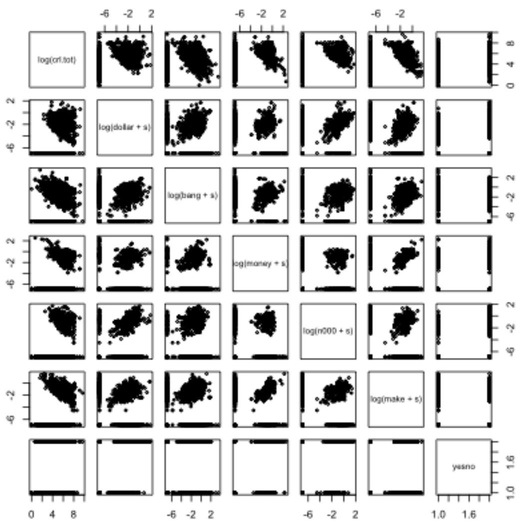
The following is a pairs plot of the variables.

```
pairs(spam, cex = 0.5)
```



It is clear from these plots that the explanatory variables are highly skewed and it is hard to see any structure in these plots. Visualization will be much easier if we take logarithms of the explanatory variables.

```
s = 0.001
pairs(~log(crl.tot) + log(dollar + s) + log(bang +
    s) + log(money + s) + log(n000 + s) + log(make +
    s) + yesno, data = spam, cex = 0.5)
```



We now fit a logistic regression model for *yesno* based on the logged explanatory variables.

```r
spam.glm <- glm(yesno ~ log(crl.tot) + log(dollar +
    s) + log(bang + s) + log(money + s) + log(n000 +
    s) + log(make + s), family = binomial, data = spam)
summary(spam.glm)
```

```
##
## Call:
## glm(formula = yesno ~ log(crl.tot) + log(dollar + s) + log(bang +
##     s) + log(money + s) + log(n000 + s) + log(make + s), family = binomial,
##     data = spam)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -3.1657  -0.4367  -0.2863   0.3609   2.7152
##
## Coefficients:
##                   Estimate Std. Error z value Pr(>|z|)
## (Intercept)        4.11947    0.36342  11.335  < 2e-16 ***
## log(crl.tot)       0.30228    0.03693   8.185 2.71e-16 ***
## log(dollar + s)    0.32586    0.02365  13.777  < 2e-16 ***
## log(bang + s)      0.40984    0.01597  25.661  < 2e-16 ***
## log(money + s)     0.34563    0.02800  12.345  < 2e-16 ***
## log(n000 + s)      0.18947    0.02931   6.463 1.02e-10 ***
## log(make + s)     -0.11418    0.02206  -5.177 2.25e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 6170.2  on 4600  degrees of freedom
## Residual deviance: 3245.1  on 4594  degrees of freedom
## AIC: 3259.1
##
## Number of Fisher Scoring iterations: 6
```

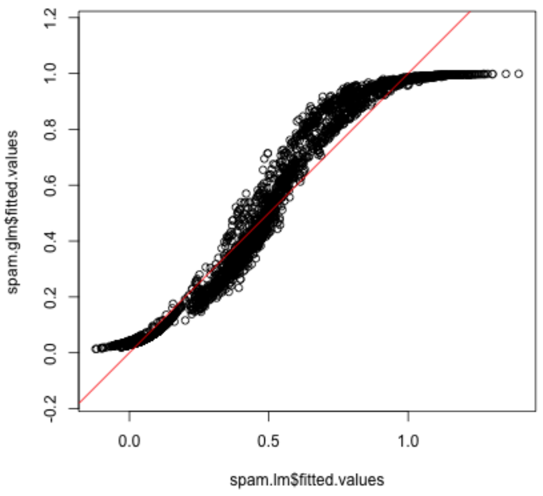
Note that all the variables are significant. We actually could have fitted a linear model as well (even though the response variable is binary).

```r
spam.lm <- lm(as.numeric(yesno == "y") ~ log(crl.tot) +
    log(dollar + s) + log(bang + s) + log(money + s) +
    log(n000 + s) + log(make + s), data = spam)
summary(spam.lm)
```

```
##
## Call:
## lm(formula = as.numeric(yesno == "y") ~ log(crl.tot) + log(dollar +
##     s) + log(bang + s) + log(money + s) + log(n000 + s) + log(make +
##     s), data = spam)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.10937 -0.13830 -0.05674  0.15262  1.05619
##
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)      1.078531   0.034188  31.547  < 2e-16 ***
## log(crl.tot)     0.028611   0.003978   7.193 7.38e-13 ***
## log(dollar + s)  0.054878   0.002934  18.703  < 2e-16 ***
## log(bang + s)    0.064522   0.001919  33.619  < 2e-16 ***
## log(money + s)   0.039776   0.002751  14.457  < 2e-16 ***
## log(n000 + s)    0.018530   0.002815   6.582 5.16e-11 ***
## log(make + s)   -0.017380   0.002370  -7.335 2.61e-13 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3391 on 4594 degrees of freedom
## Multiple R-squared:  0.5193,Adjusted R-squared:  0.5186
## F-statistic: 827.1 on 6 and 4594 DF,  p-value: < 2.2e-16
```

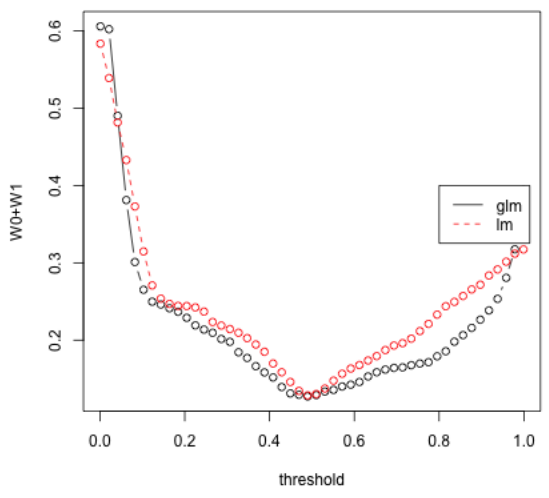
A comparison plot of the fitted values for the linear regression and logistic regression is given below.

```
par(mfrow = c(1, 1))
plot(spam.lm$fitted.values, spam.glm$fitted.values,
    asp = 1)
abline(c(0, 1), col = "red")
```



Note that some of the fitted values for the linear model are less than 0 and some are more than one. We can formally compare the prediction performance of the linear model and the generalized linear model by the confusion matrix. For various thresholds on the fitted values, the confusion matrices of linear regression and logistic regression can be computed and we can compare their misclassification error

```
v <- seq(0.001, 0.999, length = 50)
y <- as.numeric(spam$yesno == "y")
glm.conf <- confusion(y, spam.glm$fitted, v)
lm.conf <- confusion(y, spam.lm$fitted, v)
matplot(v, cbind((glm.conf[, "W1"] + glm.conf[, "W0"])/4601,
    (lm.conf[, "W1"] + lm.conf[, "W0"])/4601), xlab = "threshold",
    ylab = "W0+W1", type = "b", pch = 1)
legend(0.8, 0.4, lty = 1:2, col = 1:2, c("glm", "lm"))
```



It is clear from this plot that 0.5 is the best threshold for both linear and logistic regression as the misclassification error is minimized at 0.5. Logistic regression seems to be slightly better than linear regression at other thresholds.

5.2 Trading off different types of errors

We used the quantity $W_0 + W_1$ to quantify how many errors we make. However, these are combining together two different types of errors, and we might care about one type of error more than another. For example, if $y = 1$ if a person has a disease and $y = 0$ if they do not, then we might have different ideas about how much of the two types of error we would want. W_1 are all of the times we say someone has a disease when they don't, while W_0 is the reverse (we say someone has the disease, but they don't).

We've already seen that it's not a good idea to try to drive either W_0 or W_1 to zero (if that was our goal we could just ignore any data and always says someone has the disease, and that would make $W_0 = 0$ since we would never have $\hat{y} = 0$).

Alternatively, we might have a prediction procedure, and want to quantify how good it is, and so we want a vocabulary to talk about the types of mistakes we make.

Recall our types of results:

	pred = 0	pred = 1
obs = 0	C_0	W_1
obs = 1	W_0	C_1

There are two sets of metrics that are commonly used.

Precision/Recall

- **Precision**
  $$P(y = 1|\hat{y} = 1)$$
  We estimate it with the proportion of predictions of $\hat{y} = 1$ that are correct
  $$\frac{\#\text{ correct } \hat{y} = 1}{\#\hat{y} = 1} = \frac{C_1}{C_1 + W_1}$$
- **Recall**
  $$P(\hat{y} = 1|y = 1)$$
  Estimated with proportion of $y = 1$ that are correctly predicted
  $$\frac{\#\text{ correct } \hat{y} = 1}{\# y = 1}\frac{C_1}{C_1 + W_0}$$

Sensitivity/Specificity

- **Specificity** (or true negative rate)
  $$P(\hat{y} = 0|y = 0)$$
  Estimated with the proportion of all $y = 0$ that are correctly predicted
  $$\frac{\#\text{ correct } \hat{y} = 0}{\#\hat{y} = 0} = \frac{C_0}{C_0 + W_1}$$
- **Sensitivity** (equivalent to Recall or true positive rate)
  $$P(\hat{y} = 1|y = 1)$$
  Estimated with the proportion of all $y = 1$ that are correctly predicted
  $$\frac{\#\text{ correct } \hat{y} = 1}{\# y = 1} = \frac{C_1}{C_1 + W_0}$$

Disease classification example: If we go back to our example of $y = 1$ if a person has a disease and $y = 0$ if they do not, then we have:

- **Precision** The proportion of patients classified with the disease that actually have the disease.
- **Recall/Sensitivity** The proportion of diseased patients that will be correctly identified as diseased
- **Specificity** The proportion of non-diseased patients that will be correctly identified as non-diseased

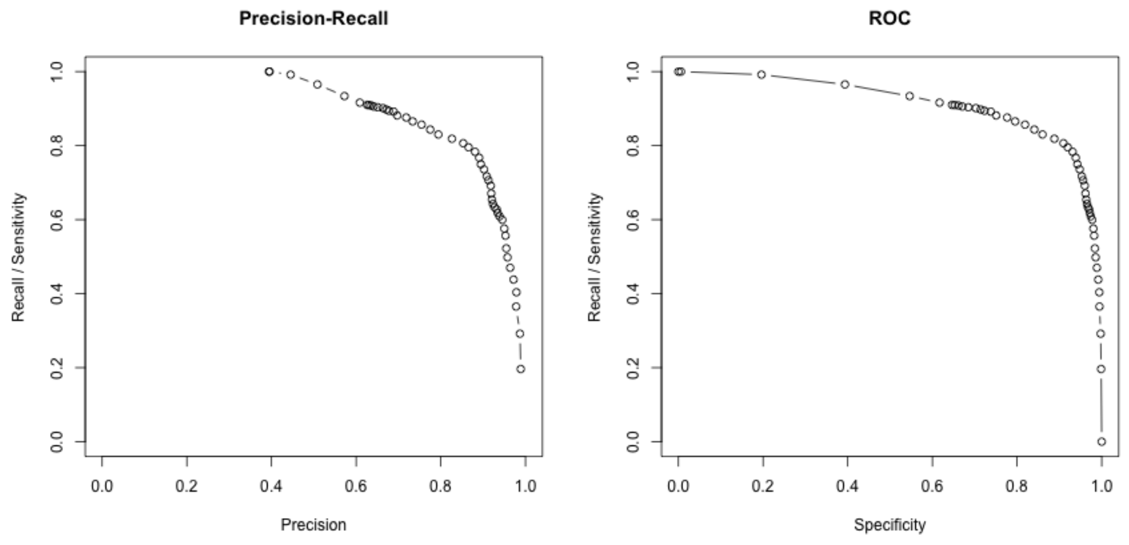
5.3 ROC/Precision-Recall Curves

These metrics come in pairs because you usually consider the two pairs together to decide on the right cutoff, as well as to generally compare techniques.

These measures are usually done plotted: Sensitivity plotted against specificity is called a ROC curve (”Receiver operating characteristic” curve); the other plot is just the precision-recall plot.

Here are these curves estimated for our glm model on the spam dataset (note that the points are where we actually evaluated it, and we draw lines between those points to get a curve)

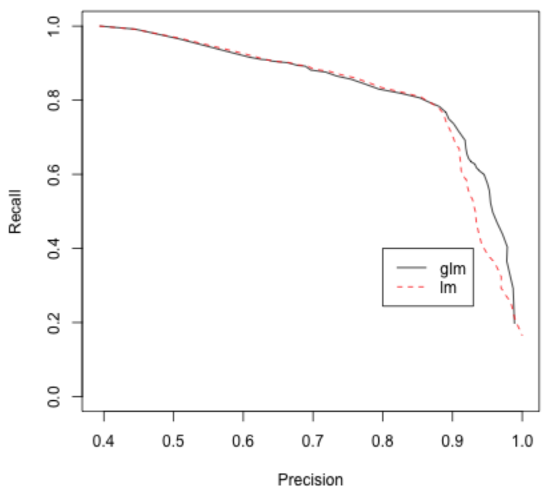
```
spamGlm.precision <- glm.conf[, "C1"]/(glm.conf[, "C1"] +
    glm.conf[, "W1"])
spamGlm.recall <- glm.conf[, "C1"]/(glm.conf[, "C1"] +
    glm.conf[, "W0"])
spamGlm.spec <- glm.conf[, "C0"]/(glm.conf[, "C0"] +
    glm.conf[, "W1"])
par(mfrow = c(1, 2))
plot(x = spamGlm.precision, y = spamGlm.recall, xlab = "Precision",
    ylab = "Recall / Sensitivity", type = "b", xlim = c(0,
        1), ylim = c(0, 1), main = "Precision-Recall")
plot(x = spamGlm.spec, y = spamGlm.recall, ylab = "Recall / Sensitivity",
    xlab = "Specificity", type = "b", xlim = c(0, 1),
    ylim = c(0, 1), main = "ROC")
```

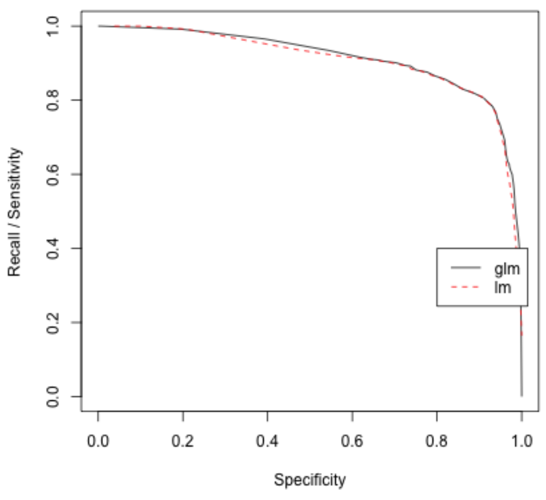


Note there is a NaN for precision for the last value of the threshold so there is no point – why would there be a NaN?

We can compare linear and logistic regressions in one plot as follows.

```
spamlm.precision <- lm.conf[, "C1"]/(lm.conf[, "C1"] +
    glm.conf[, "W1"])
spamlm.recall <- lm.conf[, "C1"]/(lm.conf[, "C1"] +
    glm.conf[, "W0"])
spamlm.spec <- lm.conf[, "C0"]/(lm.conf[, "C0"] + glm.conf[,
    "W1"])
par(mfrow = c(1, 2))
matplot(x = cbind(spamGlm.precision, spamlm.precision),
    y = cbind(spamGlm.recall, spamlm.recall), xlab = "Precision",
    ylab = "Recall", type = "l")
legend(0.8, 0.4, lty = 1:2, col = 1:2, c("glm", "lm"))
matplot(x = cbind(spamGlm.spec, spamlm.spec), y = cbind(spamGlm.recall,
    spamlm.recall), ylab = "Recall / Sensitivity",
    xlab = "Specificity", type = "l")
legend(0.8, 0.4, lty = 1:2, col = 1:2, c("glm", "lm"))
```





Why one versus the other? Notice that Precision-Recall focuses on the cases of $y = 1$ or $\hat{y} = 1$. This can be useful in cases where your focus is really on how well you detect someone and you are not concerned about how well you are detecting $y = 0$. This is most common if the vast majority of the population has $y = 0$, and you want to detect very rare events when $y = 1$ – these are often problems when you are "trying to find a needle in the haystack", and only care about your ability to find positive results. For example, suppose you want to consider how well a search engine lists of links are correctly related to the topic requested. You can imagine all websites in the world have a true $y_i = 1$ if it would be correct to be listed and the search engine gives a $\hat{y}_i = 1$ to those websites that they will return. Then precision is asking (on average) what proportion of the search engine's list of websites are correct; recall/sensitivity is asking what proportion of all of the $y_i = 1$ websites are found. Both are reasonable questions to try to trade off. Specificity, however, is what proportion of all the other (billion?) websites that are not related (i.e. $y_i = 0$) are NOT given in the search engine's list of good websites. You are not concerned about this quantity at all.

However, in other contexts it matters very much how good you are at separating the negative results (i.e. $y = 0$). Consider predicting if a patient has a disease ($\hat{y}_i = 1$), and then y_i is whether the patient actually has a disease. A negative result tells a patient that the patient doesn't have the disease – and is a serious problem if in fact the patient does have the disease, and thus doesn't get treatment.

Note that the key distinction between these two contexts the reprecussions to being negative. There are many settings where the use of the predictions is ultimately as a recommendation system (movies to see, products to buy, best times to buy something, potential important genes to investigate, etc), so mislabeling some positive things as negative (i.e. not finding them) isn't a big deal so long as what you do recommend is high quality.

Indeed, the cases where trade-offs lead to different conclusions tend to be cases where the overall proportion of $y_i = 1$ in the population is small. (However, just because they have a small proportion in the population doesn't mean you don't care about making mistakes about negatives – missing a diagnosis for a rare but serious disease is still a problem)