16. A Logistic Regression Illustration

36-402, Advanced Data Analysis

22 March 2011

The first part of lecture today was review and reinforcement of the general ideas about logistic regression and other GLMs from the previous lectures. These notes elaborate on the example I did in class, of building and testing a GLM (specifically, a logistic regression model) for a particular data set.

Specifically, we are going to build a simple weather forecaster. Our data consist of daily records, from the beginning of 1948 to the end of 1983, of precipitation at Snoqualmie Falls, Washington[1]. Each row of the data file is a different year; each column records, for that day of the year, the day's precipitation (rain or snow), in units of $\frac{1}{100}$ inch. Because of leap-days, there are 366 columns, with the last column having an NA value for three out of four years.

```
snoqualmie <- read.csv("snoqualmie.csv",header=FALSE)
snoqualmie <- unlist(snoqualmie) # Turn into one big vector without year breaks
snoqualmie <- na.omit(snoqualmie) # Remove NAs from non-leap-years
```

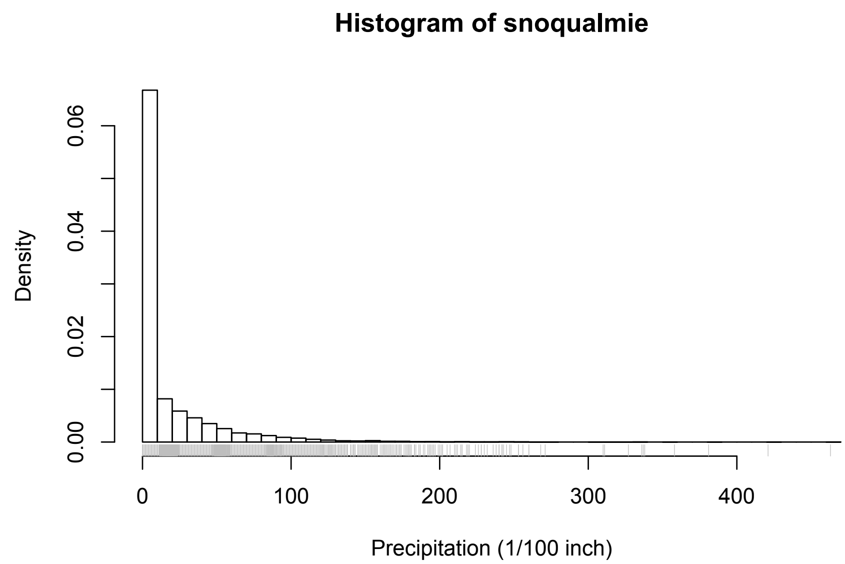
What we want to do is predict tomorrow's weather from today's. This would be of interest if we lived in Snoqualmie Falls, or if we operated either one of the local hydroelectric power plants, or the tourist attraction of the Falls themselves. Examining the distribution of the data (Figures 1 and 2) shows that there is a big spike in the distribution at zero precipitation, and that days of no precipitation can follow days of any amount of precipitation but seem to be less common after heavy precipitation.

These facts suggest that "no precipitation" is a special sort of event which would be worth predicting in its own right (as opposed to just being when the precipitation happens to be zero), so we will attempt to do so with logistic regression. Specifically, the input variable X_i will be the amount of precipitation on the i^{th} day, and the response Y_i will be the indicator variable for whether there was any precipitation on day $i+1$ — that is, $Y_i = 1$ if $X_{i+1} > 0$, an $Y_i = 0$ if $X_{i+1} = 0$. We expect from Figure 2, as well as common experience, that the coefficient on X should be positive.[2]

Before fitting the logistic regression, it's convenient to re-shape the data:

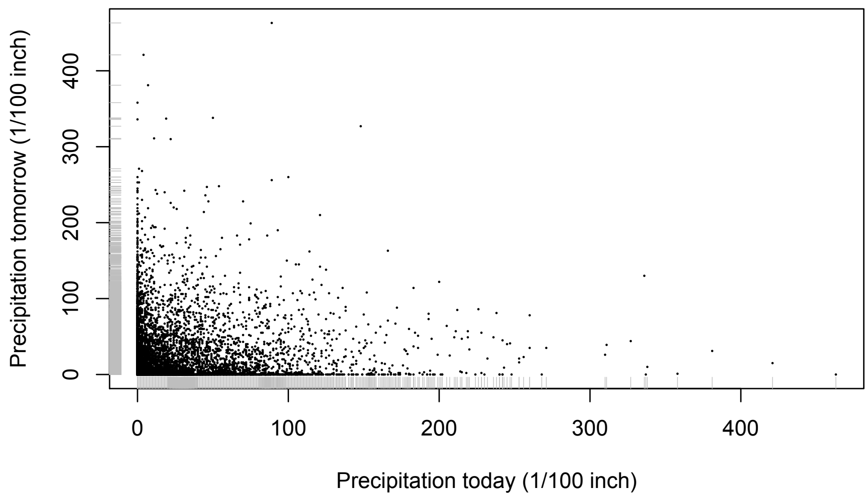
[1] I learned of this data set from Peter Guttorp's *Stochastic Modeling of Scientific Data*; the data file is available from `http://www.stat.washington.edu/peter/stoch.mod.data.html`.

[2] This does not attempt to model *how much* precipitation there will be tomorrow, if there is any. We could make that a separate model, if we can get this part right.




```
plot(hist(snoqualmie,n=50,probability=TRUE),xlab="Precipitation (1/100 inch)")
rug(snoqualmie,col="grey")
```

Figure 1: Histogram of the amount of daily precipitation at Snoqualmie Falls




```
plot(snoqualmie[-length(snoqualmie)],snoqualmie[-1],
     xlab="Precipitation today (1/100 inch)",
     ylab="Precipitation tomorrow (1/100 inch)",cex=0.1)
rug(snoqualmie[-length(snoqualmie)],side=1,col="grey")
rug(snoqualmie[-1],side=2,col="grey")
```

Figure 2: Scatterplot showing relationship between amount of precipitation on successive days. Notice that days of no precipitation can follow days of any amount of precipitation, but seem to be more common when there is little or no precipitation to start with.

```
vector.to.pairs <- function(v) {
  v <- as.numeric(v)
  n <- length(v)
  return(cbind(v[-1],v[-n]))
}
snoq.pairs <- vector.to.pairs(snoqualmie)
colnames(snoq.pairs) <- c("tomorrow","today")
snoq <- as.data.frame(snoq.pairs)
```

This creates a two-column array, where the first column is the precipitation on day $i+1$, and the second column is the precipitation on day i (hence the column names). Finally, I turn the whole thing into a data frame.

Now fitting is straightforward:

```
snoq.logistic <- glm((tomorrow > 0) ~ today, data=snoq, family=binomial)
```

To see what came from the fitting, run `summary`:

```
> summary(snoq.logistic)

Call:
glm(formula = (tomorrow > 0) ~ today, family = binomial, data = snoq)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.3713  -1.1805   0.9536   1.1693   1.1744

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) 0.0071899  0.0198430   0.362    0.717
today       0.0059232  0.0005858  10.111   <2e-16 ***
---
```

(I have cut off some uninformative bits of the output.) The coefficient on X, the amount of precipitation today, is indeed positive, and (if we can trust R's calculations) highly significant. There is also an intercept term, which is slight positive, but not very significant. We can see what the intercept term means by considering what happens when $X = 0$, i.e., on days of no precipitation. The linear predictor is then $0.0072 + 0 * (0.0059) = 0.0072$, and the predicted probability of precipitation is $e^{0.0072}/(1 + e^{0.0072}) = 0.502$. That is, even when there is no precipitation today, we predict that it is slightly more probable than not that there will be some precipitation tomorrow.[3]

We can get a more global view of what the model is doing by plotting the data and the predictions (Figure 3). This shows a steady increase in the probability of precipitation tomorrow as the precipitation today increases, though with the leveling off characteristic of logistic regression. The (approximate)

[3]For western Washington State, this is plausible — but see below.

95% confidence limits for the predicted probability are (on close inspection) asymmetric, and actually slightly narrower at the far right than at intermediate values of X (Figure).

How well does this work? We can get a first sense of this by comparing it to a simple nonparametric smoothing of the data. Remembering that when Y is binary, $\Pr Y = 1|X = x = \mathbb{E}[Y|X = x]$, we can use a smoothing spline to estimate $\mathbb{E}[Y|X = x]$ (Figure 5). This would not be so great as a model — it ignores the fact that the response is a binary event and we're trying to estimate a probability, the fact that the variance of Y therefore depends on its mean, etc. — but it's at least indicative.

The result is in not-terribly-bad agreement with the logistic regression up to about 1.2 or 1.3 inches of precipitation, after which it runs significantly below the logistic regression, rejoins it around 3.5 inches of precipitation, and then (as it were) falls off a cliff.

We can do better by fitting a generalized additive model. In this case, with only one predictor variable, this means using non-parametric smoothing to estimate the log odds — we're still using the logistic transformation, but only requiring that the log odds change smoothly with X, not that they be linear in X. The result (Figure 6) is actually quite similar to the spline, but a bit better behaved, and has confidence intervals. At the largest values of X, the latter span nearly the whole range from 0 to 1, which is not unreasonable considering the sheer lack of data there.

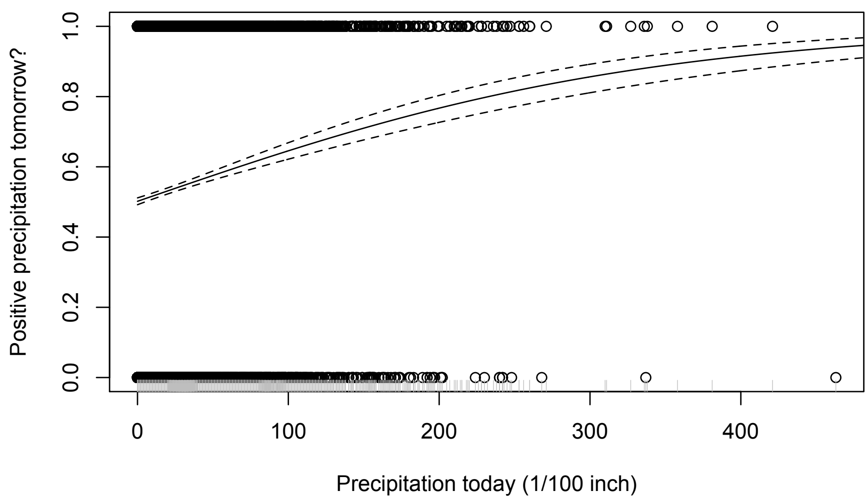
Visually, the logistic regression curve is usually but not always within the confidence limits of the non-parametric predictor. What can we say about the difference between the two models more quantiatively?

Numerically, the deviance is 18079.69 for the logistic regression, and 18036.77 for the GAM. We can go through the testing procedure outlined in the notes for lecture 14. We need a simulator (which presumes that the logistic regression model is true), and we need to calculate the difference in deviance on simulated data many times.

```
# Simulate from the fitted logistic regression model for Snoqualmie
# Presumes: fitted values of the model are probabilities.
snoq.sim <- function(model=snoq.logistic) {
  fitted.probs <- fitted(model)
  n <- length(fitted.probs)
  new.binary <- rbinom(n,size=1,prob=fitted.probs)
  return(new.binary)
}
```

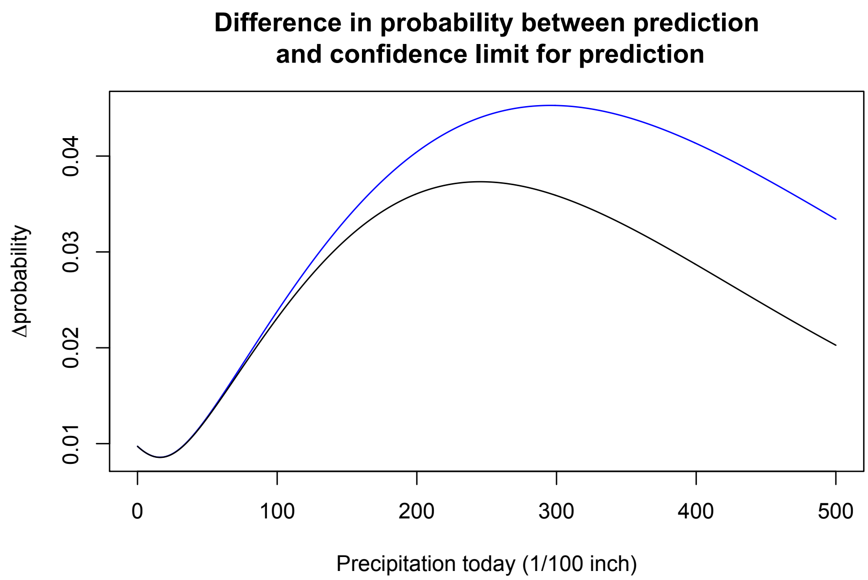
A quick check of the simulator against the observed values:

```
> summary(ifelse(snoq[,1]>0,1,0))
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
 0.0000  0.0000  1.0000  0.5262  1.0000  1.0000
> summary(snoq.sim())
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
```



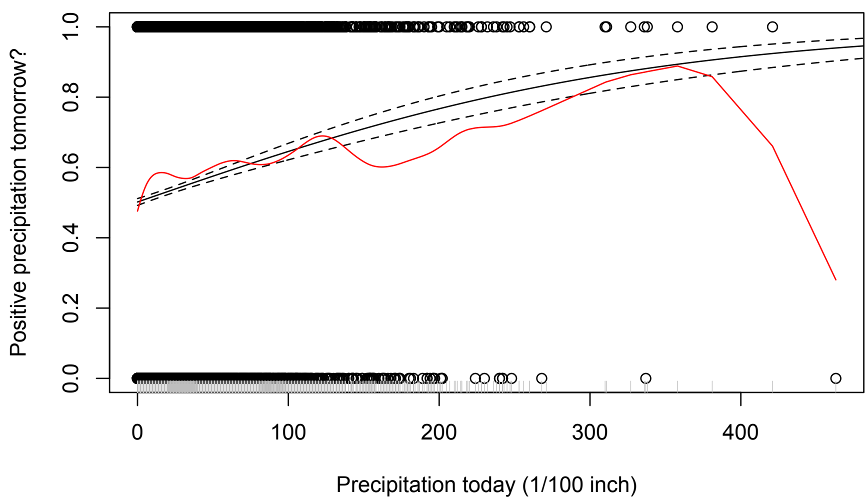

```
plot((tomorrow>0)~today,data=snoq,xlab="Precipitation today (1/100 inch)",
     ylab="Positive precipitation tomorrow?")
rug(snoq$today,side=1,col="grey")

data.plot <- data.frame(today=(0:500))
logistic.predictions <- predict(snoq.logistic,newdata=data.plot,se.fit=TRUE)
lines(0:500,ilogit(logistic.predictions$fit))
lines(0:500,ilogit(logistic.predictions$fit+1.96*logistic.predictions$se.fit),
      lty=2)
lines(0:500,ilogit(logistic.predictions$fit-1.96*logistic.predictions$se.fit),
      lty=2)
```

Figure 3: Data (dots), plus predicted probabilities (solid line) and approximate 95% confidence intervals from the logistic regression model (dashed lines). Note that calculating standard errors for predictions on the logit scale, and then transforming, is better practice than getting standard errors directly on the probability scale.



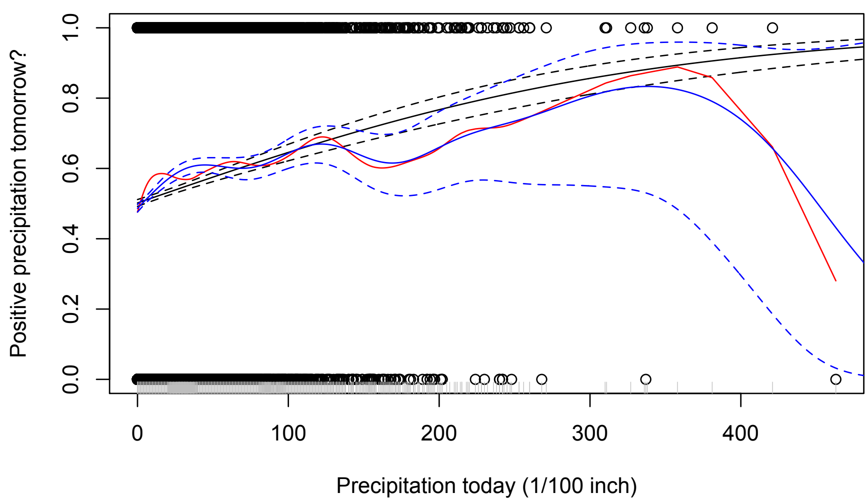

```
plot(0:500,ilogit(logistic.predictions$fit)
           -ilogit(logistic.predictions$fit-1.96*logistic.predictions$se.fit),
    type="l",col="blue",xlab="Precipitation today (1/100 inch)",
    main="Difference in probability between prediction\n
and confidence limit for prediction",
    ylab = expression(paste(Delta,"probability")))
lines(0:500,ilogit(logistic.predictions$fit+1.96*logistic.predictions$se.fit)
            -ilogit(logistic.predictions$fit))
```

Figure 4: Distance from the fitted probability to the upper (black) and lower (blue) confidence limits. Notice that the two are not equal, and somewhat smaller at very large values of X than at intermediate ones. (Why?)




```
snoq.spline <- smooth.spline(x=snoq$today,y=(snoq$tomorrow>0))
lines(snoq.spline,col="red")
```

Figure 5: As Figure 3, plus a smoothing spline (red).




```
library(mgcv)
snoq.gam <- gam((tomorrow>0)~s(today),data=snoq,family=binomial)
gam.predictions <- predict.gam(snoq.gam,newdata=data.plot,se.fit=TRUE)
lines(0:500,ilogit(gam.predictions$fit),col="blue")
lines(0:500,ilogit(gam.predictions$fit+1.96*gam.predictions$se.fit),
      col="blue",lty=2)
lines(0:500,ilogit(gam.predictions$fit-1.96*gam.predictions$se.fit),
      col="blue",lty=2)
```

Figure 6: As Figure 5, but with the addition of a generalized additive model (blue line) and its confidence limits (dashed blue lines). *Note:* the `predict` function in the `gam` package does not allow one to calculate standard errors for new data. You may need to un-load the `gam` library first, with `detach(package:gam)`.

```
 0.0000  0.0000  1.0000  0.5264  1.0000  1.0000
```

This suggests that the simulator is not acting crazily.

Now for the difference in deviances:

```
# Simulate from fitted logistic regression, re-fit logistic regression and
# GAM, calculate difference in deviances
diff.dev <- function(model=snoq.logistic,x=snoq[,2]) {
  y.new <- snoq.sim(model)
  GLM.dev <- glm(y.new ~ x,family=binomial)$deviance
  GAM.dev <- gam(y.new ~ s(x),family=binomial)$deviance
  return(GLM.dev-GAM.dev)
}
```

A single run of this takes about 1.5 seconds on my computer.

Finally, we calculate the distribution of difference in deviances under the null (that the logistic regression is properly specified), and the corresponding p-value:

```
diff.dev.obs <- snoq.logistic$deviance - snoq.gam$deviance
null.dist.of.diff.dev <- replicate(1000,diff.dev())
p.value <- (1+sum(null.dist.of.diff.dev > diff.dev.obs))/(1+length(null.dist.of.diff.dev))
```

Using a thousand replicates takes about 1500 seconds, or roughly 25 minutes, which is substantial, but not impossible; it gave a p-value of $< 10^{-3}$, and the following sampling distribution:

```
> summary(null.dist.of.diff.dev)
     Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
 0.000097  0.002890  0.016770  2.267000  2.897000 29.750000
```

(A preliminary trial run of only 100 replicates, taking a few minutes, gave

```
> summary(null.dist.of.diff.dev)
     Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
 0.000291  0.002681  0.013700  2.008000  2.121000 27.820000
```

which implies a p-value of < 0.01. This would be good enough for many practical purposes.)

Having detected that there is a problem with the GLM, we can ask where it lies. We *could* just use the GAM, but it's more interesting to try to diagnose what's going on.

In this respect Figure 6 is actually a little misleading, because it leads the eye to emphasize the disagreement between the models at large X, when actually there are very few data points there, and so even large differences in predicted probabilities there contribute little to the over-all likelihood difference. What is actually more important is what happens at $X = 0$, which contains a very large number of observations (about 47% of all observations), and which we have reason to think is a special value anyway.

Let's try introducing a dummy variable for $X = 0$ into the logistic regression, and see what happens. It will be convenient to augment the data frame with an extra column, recording 1 whenever $X = 0$ and 0 otherwise.

```
snoq2 <- data.frame(snoq,dry=ifelse(snoq$today==0,1,0))
snoq2.logistic <- glm((tomorrow > 0) ~ today + dry,data=snoq2,family=binomial)
snoq2.gam <- gam((tomorrow > 0) ~ s(today) + dry,data=snoq2,family=binomial)
```

Notice that I allow the GAM to treat zero as a special value as well, by giving it access to that dummy variable. In principle, with enough data it can decide whether or not that is useful on its own, but since we have guessed that it is, we might as well include it. Figure 7 shows the data and the two new models. These are *extremely* close to each other. The new GLM has a deviance of 18015.65, lower than even the GAM before, and the new GAM has a deviance of 18015.21. The p-value is essentially 1 — and yet we know that the test, with this test, *does* have power to detect departures from the parametric model. This is very promising.

Let's turn now to looking at calibration. The actual fraction of no-precipitation days which are followed by precipitation is

```
> mean(snoq$tomorrow[snoq$today==0]>0)
[1] 0.4702199
```

What does the new logistic model predict?

```
> predict(snoq2.logistic,newdata=data.frame(today=0,dry=1),type="response")
        1
0.4702199
```

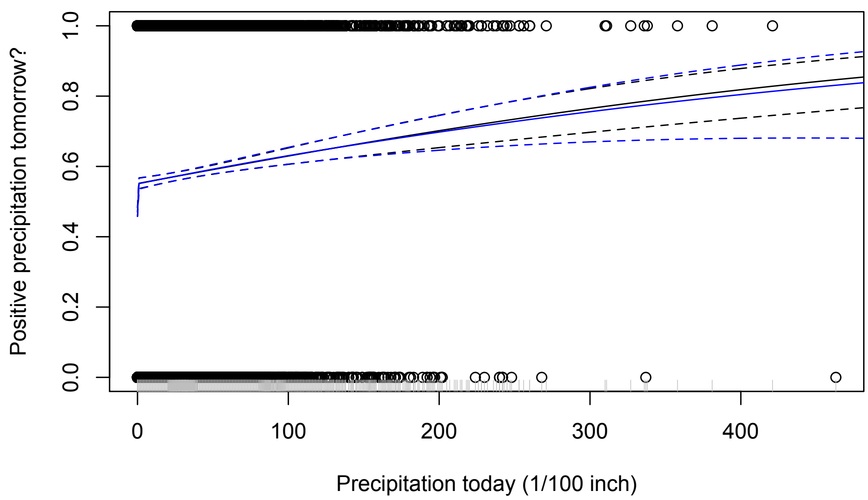
This should not be surprising — we've given the model a special parameter dedicated to getting this one probability exactly right! The hope however is that this will change the predictions made on days *with* precipitation so that they are better.

We'll tackle this through calibration. Looking at a histogram of fitted values (`hist(fitted(snoq2.logistic))`) shows a gap in the distribution of predicted probabilities between 0.47 and about 0.55, so we'll look first at days where the predicted probability is between 0.55 and 0.56.

```
> mean(snoq$tomorrow[(fitted(snoq2.logistic) >= 0.55)
                     & (fitted(snoq2.logistic) < 0.56)] > 0)
[1] 0.5474882
```

Not bad — but a bit painful to write out. Let's write a function.

```
frequency.vs.probability <- function(p.lower,p.upper=p.lower+0.01,
                                     model=snoq2.logistic,
                                     data=(snoq$tomorrow>0)) {
  fitted.probs <- fitted(model)
  indices <- (fitted.probs >= p.lower) & (fitted.probs < p.upper)
```




```
plot((tomorrow>0)~today,data=snoq,xlab="Precipitation today (1/100 inch)",
     ylab="Positive precipitation tomorrow?")
rug(snoq$today,side=1,col="grey")

data.plot=data.frame(data.plot,dry=ifelse(data.plot$today==0,1,0))
logistic.predictions2 <- predict(snoq2.logistic,newdata=data.plot,se.fit=TRUE)
lines(0:500,ilogit(logistic.predictions2$fit))
lines(0:500,ilogit(logistic.predictions2$fit+1.96*logistic.predictions2$se.fit),
      lty=2)
lines(0:500,ilogit(logistic.predictions2$fit-1.96*logistic.predictions2$se.fit),
      lty=2)
gam.predictions2 <- predict.gam(snoq2.gam,newdata=data.plot,se.fit=TRUE)
lines(0:500,ilogit(gam.predictions2$fit),col="blue")
lines(0:500,ilogit(gam.predictions2$fit+1.96*gam.predictions2$se.fit),
      col="blue",lty=2)
lines(0:500,ilogit(gam.predictions2$fit-1.96*gam.predictions2$se.fit),
      col="blue",lty=2)
```

Figure 7: As Figure 6, but allowing the two models to use a dummy variable indicating when today is completely dry ($X = 0$).

```
  ave.prob <- mean(fitted.probs[indices])
  frequency <- mean(data[indices])
  se <- sqrt(ave.prob*(1-ave.prob)/sum(indices))
  out <- list(frequency=frequency,ave.prob=ave.prob,se=se)
  return(out)
}
```

I have added a calculation of the average predicted probability, and a crude estimate of the standard error we should expect if the observations really are binomial with the predicted probabilities[4]. Try the function out before doing anything rash:

```
> frequency.vs.probability(0.55)
$frequency
[1] 0.5474882

$ave.prob
[1] 0.5548081

$se
[1] 0.00984567
```

This agrees with our previous calculation.

Now we can do this for a lot of probability brackets:

```
f.vs.p <- sapply((55:74)/100,frequency.vs.probability)
```

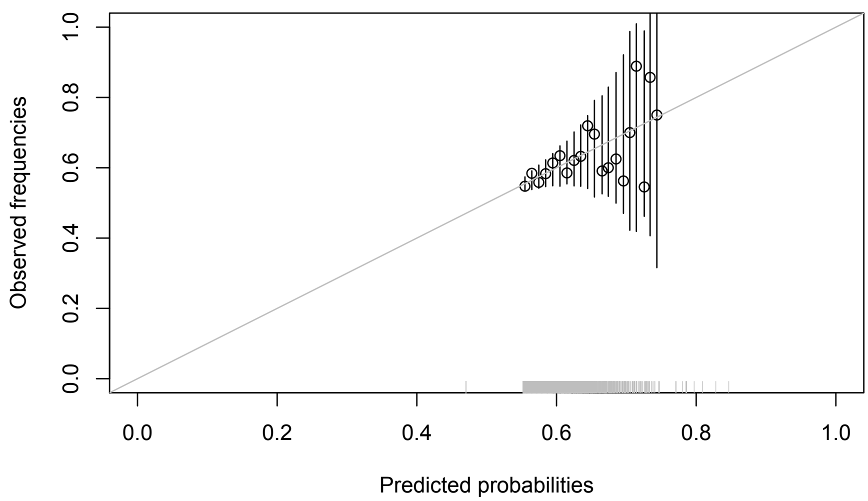
This comes with some unfortunate R cruft, removable thus

```
f.vs.p <- data.frame(frequency=unlist(f.vs.p["frequency",]),
                     ave.prob=unlist(f.vs.p["ave.prob",]),
                     se=unlist(f.vs.p["se",]))
```

and we're ready to plot (Figure 8). The observed frequencies are generally quite near to the predicted probabilites, especially when the number of observations is large and so the sample frequency *should* be close to the true probability. While I wouldn't want to say this was the last word in weather forecasting[5], it's surprisingly good for such a simple model.

[4] This could be improved by averaging predicted variances for each point, but using probability ranges of 0.01 makes it hardly worth the effort.

[5] There is an extensive discussion of this data in chapter 2 of Guttorp's book, including many significant refinements, such as dependence across multiple days.




```
plot(f.vs.p$ave.prob,f.vs.p$frequency,xlim=c(0,1),ylim=c(0,1),
     xlab="Predicted probabilities",ylab="Observed frequencies")
rug(fitted(snoq2.logistic),col="grey")
abline(0,1,col="grey")
segments(x0=f.vs.p$ave.prob,y0=f.vs.p$ave.prob-1.96*f.vs.p$se,
         y1=f.vs.p$ave.prob+1.96*f.vs.p$se)
```

Figure 8: Calibration plot for the modified logistic regression model `snoq2.logistic`. Points show the actual frequency of precipitation for each level of predicted probability. Vertical lines are (approximate) 95% sampling intervals for the frequency, given the predicted probability and the number of observations.