

Logistic Regression Example

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Abstract

This examples demonstrates the `binaryReg` and other logistic regression support functions in the `smwrStats` package. The example uses the PugetNitrate dataset from Tesoriero and Voss (1997). The dataset is available from the `smwrData` package.

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1 Introduction

These examples use data from the smwrData package. The data are retrieved in the following code.

```
> # Load the smwrStats and smwrData packages
> library(smwrStats)
> library(smwrData)
> # Get the dataset
> data(PugetNitrate)
> head(PugetNitrate)

  wellid      110      120      140 surfgeo       date nitrate
1 1000 15.375154 0.000000 57.687577 Coarse 1990-09-06    0.2
2 1001  7.839196 77.185930  9.849246 Coarse 1993-06-17    9.4
3 1002  7.236181 35.276382 53.969849 Coarse 1991-05-14    0.4
4 1003 34.472362 11.155779 53.668342 Coarse 1992-05-11   1.0
5 1004  4.623116 13.869347 81.507538 Alluvium 1989-03-17    0.2
6 1005 54.974874  0.201005 21.507538 Coarse 1988-09-19    2.8

  wellmet
1 60.9600
2  5.4864
3 21.9456
4 113.9952
5 30.1752
6 16.7640
```

2 Single Variable Model

The `hosmerLemeshow.test`, `leCessie.test`, and `roc` functions performs diagnostic tests on a logistic regression model created by `glm`. The model can be constructed from either discrete values or counts of successes and failures.

This example follows the assumptions in Tesoriero and Voss (1997). The regression will model the probability that the concentration equals or exceeds 3 mg/L as was done in that report. This example demonstrates the `hosmerLemeshow.test` and `roc` functions on one single variable model described by Tesoriero and Voss (1997). The `leCessie.test` is useful for `glm` models with fewer than 1000 observations because of the time required to process larger sample sizes.

```
> # Create the logistic regression model
> PSN03.1 <- glm(formula = nitrate >= 3 ~ wellmet, family = binomial,
+   data = PugetNitrate, na.action = na.exclude)
> # Print the summary
> print(summary(PSN03.1))

Call:
glm(formula = nitrate >= 3 ~ wellmet, family = binomial, data = PugetNitrate,
     na.action = na.exclude)

Deviance Residuals:
    Min      1Q  Median      3Q      Max
-0.7066 -0.4635 -0.3338 -0.1904  3.0984

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.224334  0.161778 -7.568 3.79e-14 ***
wellmet      -0.029482  0.003857 -7.644 2.10e-14 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 1014.85 on 1966 degrees of freedom
Residual deviance: 925.19 on 1965 degrees of freedom
AIC: 929.19

Number of Fisher Scoring iterations: 7
```

The statistics from the printed summary agree reasonably well with table 2 in Tesoriero and Voss (1997). Small differences can be expected among different

logistic regression implementations due to differences in convergence criteria for example. The G statistics in table 2 is the difference between the null deviance and the model deviance, $1014.85 - 925.19 = 89.66$.

The `hosmerLemeshow.test` can help diagnose lack of fit and the output can help construct diagnostic plots like figure 2 in Tesoriero and Voss (1997). The code below runs the test and creates a graph to replicate figure 2, very small differences can be noted due to small differences in grouping.

```
> # Run the H-L test
> PSN03.1.hl <- hosmerLemeshow.test(PSN03.1)
> print(PSN03.1.hl)

Hosmer-Lemeshow goodness of fit test

data: nitrate >= 3 ~ wellmet
Chi-square = 22.437, Number of groups = 10, p-value = 0.004167
alternative hypothesis: Some lack of fit
null hypothesis: No lack of fit
sample estimates:
      Size Expected Counts    wellmet
1 196     0.751        1 172.67231
2 199     2.965        3 101.52597
3 193     4.917       12  82.38760
4 206     8.104        8  67.11370
5 191    10.476        5  55.11933
6 188    12.848       14  47.14186
7 203    17.736       10  38.15706
8 199    21.979       16  29.28531
9 196    26.677       28  21.22714
10 196   34.547       44  10.89038

> # Added fitted values to dataset for line in figure 2, and order
> PugetNitrate$fits <- fitted(PSN03.1)
> OrderFits <- order(PugetNitrate$fits)
> # setSweave is a specialized function that sets up the graphics page for
> # Sweave scripts. For interactive use, it should be removed and the
> # default setting for set.up can be used.
> setSweave("binplot01", 5, 5)
> with(PugetNitrate, xyPlot(wellmet[OrderFits], fits[OrderFits],
+   Plot=list(what="lines"),
+   xaxis.range=c(0, 200),
+   yaxis.range=c(0, .25),
+   xtitle="Well Depth, in meters",
+   ytitle="Estimated Pobability"))
> # Add the observed frequencies
```

```

> with(PSN03.1.hl$estimate, addXY(wellmet, Counts/Size,
+   Plot=list(what="points")))
> # Required call to close PDF output graphics
> graphics.off()

```

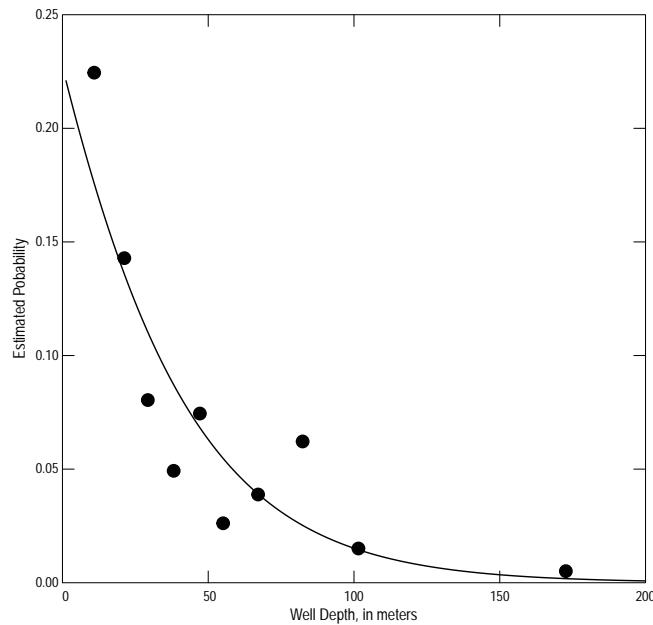


Figure 1. The estimated probability that nitrate exceeds 3 mg/L as a function of well depth.

The Hosmer-Lemeshow test can be very sensitive to the number of groups. Compare the p-values from the previous test using the default 10 groups with the output below for 12 groups.

```

> # Run the H-L test with 12 groups
> hosmerLemeshow.test(PSN03.1, 12)

```

Hosmer-Lemeshow goodness of fit test

```

data: nitrate >= 3 ~ wellmet
Chi-square = 15.603, Number of groups = 12, p-value = 0.1116
alternative hypothesis: Some lack of fit
null hypothesis: No lack of fit

```

```

sample estimates:
  Size Expected Counts    wellmet
1   162      0.466       0 183.632593
2   162      1.942       3 109.071363
3   171      3.567       7  89.258274
4   160      4.906       7  75.763755
5   166      7.160       7  63.725234
6   164      9.171       5  54.388215
7   162     10.901      10  47.688030
8   172     14.207      12  40.208791
9   157     15.984       9  32.365101
10  160     19.137      21  26.216610
11  173     24.963      22  18.911695
12  158     28.596      38  9.761316

```

Another quick evaluation of a logistic regression is the area under the receiver-operating-curve (AUROC). It is a measure of the predictive power of the model. The result is a number from varies from 0.5, no predictive power, to 1.0, perfect prediction. Take, from <http://gim.unmc.edu/dxtests/Default.htm>, accessed on 01/27/2009, gives general guidelines for the AUROC: .50-.60, fail; .60-70, poor; .70-80, fair, .80-.90 good, and .90-1.00 excellent. The `roc` function computes the statistic for any model. The output from the single variable model is shown below. The result indicates fair prediction.

```

> # Compute the area under the ROC
> roc(PSN03.1)

```

Area under the ROC curve: 0.732

3 Multiple Variable Model

The `binaryReg` function performs a series of diagnostic tests on a logistic regression model created by `glm`. The model can be constructed from either discrete values or counts of successes and failures.

This example follows the assumptions in Tesoriero and Voss (1997) for the groundwater vulnerability model for coarse-grained glacial materials. The regression will model the probability that the concentration equals or exceeds 3 mg/L as was done in that report. This example demonstrates the `binaryReg` function.

```
> # Create the logistic regression model
> PSN03.3 <- glm(formula = nitrate >= 3 ~ wellmet + 120 + 110,
+   family = binomial, subset = surfgeo == "Coarse",
+   data = PugetNitrate, na.action = na.omit)
> # Create the assessment and print it
> PSN03.3.br <- binaryReg(PSN03.3)
> print(PSN03.3.br)

Call:
glm(formula = nitrate >= 3 ~ wellmet + 120 + 110, family = binomial,
     data = PugetNitrate, subset = surfgeo == "Coarse", na.action = na.omit)

Deviance Residuals:
    Min      1Q      Median      3Q      Max
-1.5005 -0.4720 -0.3274 -0.1869  3.0998

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -2.067279  0.340674 -6.068 1.29e-09 ***
wellmet     -0.028260  0.005854 -4.827 1.38e-06 ***
120         0.033697  0.006033  5.586 2.33e-08 ***
110         0.029039  0.006281  4.624 3.77e-06 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 518.48 on 718 degrees of freedom
Residual deviance: 409.71 on 715 degrees of freedom
(23 observations deleted due to missingness)
AIC: 417.71

Number of Fisher Scoring iterations: 6
```

```
Likelihood ratio test: 108.772 on 3 degrees of freedom, p-value is 0
```

```
Response profile:
```

	nitrate >= 3	Response	Counts
1	FALSE	0	635
2	TRUE	1	84

```
Goodness of fit tests
```

```
le Cessie-van Houwelingen GOF test
```

```
data: nitrate >= 3 ~ wellmet + 120 + 110
Chisq = 22.876, df = 13.509, p-value = 0.0523
alternative hypothesis: Some lack of fit
null hypothesis: No lack of fit
sample estimates:
      Q      E[Q]      se[Q]
58.56150 34.58332 13.30655
```

```
Distance between observations:
```

	maximum bandwidth
	6.237748 1.471405

```
Hosmer-Lemeshow goodness of fit test
```

```
data: nitrate >= 3 ~ wellmet + 120 + 110
Chi-square = 1.7, Number of groups = 10, p-value = 1
alternative hypothesis: Some lack of fit
null hypothesis: No lack of fit
sample estimates:
      Size Expected Counts
1     72      0.460      1
2     72      1.408      2
3     72      2.329      2
4     72      3.326      3
5     72      4.335      4
6     71      5.612      5
7     72      7.332      7
8     72      9.566      8
9     72     14.846     15
10    72     34.786     37
```

```
Predictive power estimates:
```

McFadden R-squared: 0.2098
adjusted R-squared: 0.1982

Classification table.
Percent correct: (1 is sensitivity, 0 is specificity)
1 0
25.0 97.8

Concordance Index, based on 53340 pairs
Discordant Tied Concordant
18.830146 0.001875 81.167979

Area under the ROC curve: 0.812

Influence diagnostic test criteria:
leverage cooksD dfits
0.02086 0.89220 0.34745

Observations exceeding at least one test criterion

	X...nitrate.X3	yhat	resids	deviance.res	pearson.res	leverage
2	TRUE	0.6471	0.3529	0.9330	0.7385	0.026464*
16	TRUE	0.3369	0.6631	1.4752	1.4030	0.009688
70	FALSE	0.6556	-0.6556	-1.4600	-1.3796	0.025465*
209	FALSE	0.6308	-0.6308	-1.4117	-1.3071	0.026157*
324	TRUE	0.5081	0.4919	1.1637	0.9839	0.041930*
345	TRUE	0.4948	0.5052	1.1862	1.0104	0.016866
465	FALSE	0.4309	-0.4309	-1.0618	-0.8701	0.024294*
475	FALSE	0.6252	-0.6252	-1.4010	-1.2916	0.038238*
503	TRUE	0.6516	0.3484	0.9256	0.7312	0.025533*
564	TRUE	0.5712	0.4288	1.0584	0.8665	0.021289*
578	FALSE	0.6716	-0.6716	-1.4923	-1.4300	0.027909*
584	FALSE	0.5343	-0.5343	-1.2362	-1.0711	0.022086*
599	FALSE	0.5801	-0.5801	-1.3174	-1.1754	0.022359*
643	FALSE	0.3427	-0.3427	-0.9161	-0.7220	0.021726*
687	TRUE	0.6792	0.3208	0.8795	0.6872	0.030449*
710	FALSE	0.3150	-0.3150	-0.8699	-0.6781	0.009529
732	FALSE	0.6756	-0.6756	-1.5005	-1.4431	0.024312*
733	TRUE	0.6718	0.3282	0.8920	0.6990	0.024399*
734	FALSE	0.6545	-0.6545	-1.4579	-1.3763	0.024823*
1106	FALSE	0.6027	-0.6027	-1.3587	-1.2317	0.021197*
1149	TRUE	0.6069	0.3931	0.9994	0.8048	0.023333*
1298	TRUE	0.5932	0.4068	1.0220	0.8282	0.025341*
1302	FALSE	0.6519	-0.6519	-1.4527	-1.3683	0.024970*
1407	FALSE	0.3451	-0.3451	-0.9202	-0.7260	0.011029
1429	TRUE	0.6115	0.3885	0.9917	0.7970	0.029121*

1499	FALSE	0.4160	-0.4160	-1.0372	-0.8440	0.032769*
1517	TRUE	0.4799	0.5201	1.2118	1.0411	0.038195*
1518	FALSE	0.4863	-0.4863	-1.1542	-0.9730	0.038610*
1524	FALSE	0.5722	-0.5722	-1.3032	-1.1566	0.024865*
1535	TRUE	0.6894	0.3106	0.8625	0.6713	0.026537*
1628	FALSE	0.5952	-0.5952	-1.3448	-1.2125	0.025310*
1629	TRUE	0.6558	0.3442	0.9187	0.7245	0.031254*
1748	FALSE	0.3710	-0.3710	-0.9630	-0.7680	0.032507*
1775	FALSE	0.1171	-0.1171	-0.4991	-0.3642	0.022628*
1776	TRUE	0.4444	0.5556	1.2736	1.1181	0.040658*
1777	FALSE	0.1137	-0.1137	-0.4913	-0.3582	0.022933*
1780	FALSE	0.1486	-0.1486	-0.5672	-0.4178	0.025516*
1781	TRUE	0.3834	0.6166	1.3847	1.2683	0.037391*
1782	FALSE	0.2802	-0.2802	-0.8109	-0.6240	0.030746*
1850	FALSE	0.4639	-0.4639	-1.1166	-0.9302	0.038909*
1904	TRUE	0.5667	0.4333	1.0658	0.8745	0.022855*
1935	TRUE	0.3890	0.6110	1.3741	1.2532	0.010635
	cooksD		dfits			
2	4.819e-02	-0.440932*				
16	3.310e-02	0.367118*				
70	7.237e-02	-0.541882*				
209	2.313e-02	-0.304688				
324	6.783e-03	-0.164669				
345	3.249e-02	0.362151*				
465	1.002e-02	0.200280				
475	1.303e-02	-0.228315				
503	6.426e-02	-0.510145*				
564	1.799e-03	0.084783				
578	1.109e-01	-0.672834*				
584	2.076e-02	0.288699				
599	1.255e-04	0.022392				
643	1.585e-02	0.252151				
687	1.484e-01	-0.780348*				
710	3.004e-02	0.349483*				
732	1.232e-01	-0.711441*				
733	1.123e-01	-0.678452*				
734	6.962e-02	-0.531418*				
1106	4.581e-03	-0.135351				
1149	4.907e-03	-0.140079				
1298	2.246e-04	-0.029952				
1302	6.156e-02	-0.499263*				
1407	4.081e-02	0.407956*				
1429	9.471e-03	-0.194669				
1499	7.507e-03	0.173268				
1517	1.975e-05	-0.008882				
1518	3.318e-04	-0.036405				

1524	3.405e-03	0.116667
1535	1.788e-01	-0.861079*
1628	2.732e-04	-0.033035
1629	7.783e-02	-0.561383*
1748	7.957e-03	0.178396
1775	1.879e-02	-0.274550
1776	1.497e-03	0.077341
1777	1.880e-02	-0.274683
1780	1.562e-02	-0.250167
1781	6.383e-03	0.159745
1782	3.558e-04	0.037698
1850	3.632e-04	0.038091
1904	4.133e-03	0.128556
1935	3.819e-02	0.394507*

References

- [1] Tesoriero, A.J., and Voss, F.D., 1997, Predicting the probability of elevated nitrate concentrations in the Puget Sound Basin???Implications for aquifer susceptibility and vulnerability: Groundwater, v. 35, no. 6, p. 1029???1039.
- [2] Helsel, D.R. and Hirsch, R.M., 2002, Statistical methods in water resources: U.S. Geological Survey Techniques of Water-Resources Investigations, book 4, chap. A3, 522 p.