

# 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.

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Single Variable Model</b>	<b>3</b>
<b>3</b>	<b>Multiple Variable Model</b>	<b>7</b>

# 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	wellmet
1	1000	15.375154	0.000000	57.687577	Coarse	1990-09-06	0.2	60.9600
2	1001	7.839196	77.185930	9.849246	Coarse	1993-06-17	9.4	5.4864
3	1002	7.236181	35.276382	53.969849	Coarse	1991-05-14	0.4	21.9456
4	1003	34.472362	11.155779	53.668342	Coarse	1992-05-11	1.0	113.9952
5	1004	4.623116	13.869347	81.507538	Alluvium	1989-03-17	0.2	30.1752
6	1005	54.974874	0.201005	21.507538	Coarse	1988-09-19	2.8	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)

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.

```

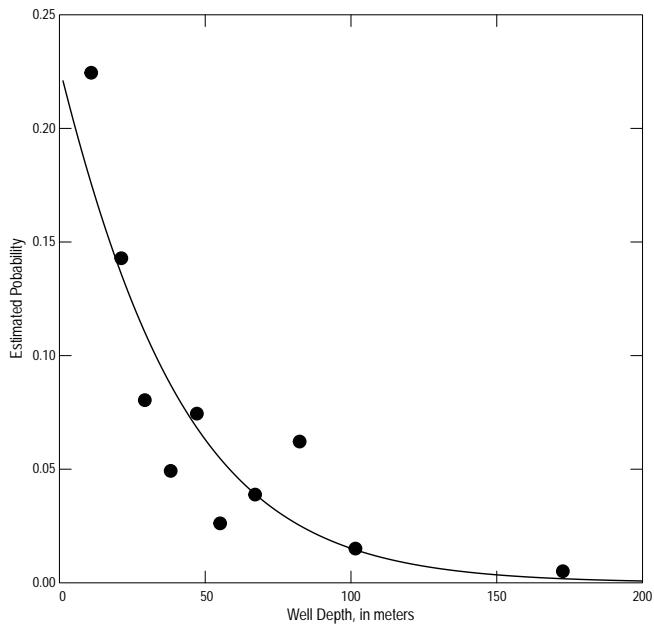
> # Run the H-L test
> PSN03.1.hl <- hosmerLemeshow.test(PSN03.1)
> print(PSN03.1.hl)

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 + l20 + l10,
+   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 + l20 + l10, family = binomial,
     data = PugetNitrate, subset = surfgeo == "Coarse", na.action = na.omit)

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 ***
l20          0.033697  0.006033  5.586 2.33e-08 ***
l10          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.