Stat 306: Finding Relationships in Data. Lecture 19 6.2 Logistic regression (Part 2)

From last lecture, we have three equivalent ways to write out the logistic regression model:

$$log\left(\frac{Pr(Y=1|\mathbf{X}=\mathbf{x})}{Pr(Y=0|\mathbf{X}=\mathbf{x})}\right) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$

$$\frac{Pr(Y=1|\mathbf{X}=\mathbf{x})}{Pr(Y=0|\mathbf{X}=\mathbf{x})} = e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}$$

$$Pr(Y = 1 | \mathbf{X} = \mathbf{x}) = \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}}$$

Recall that: k is the number of β 's (here p + 1)

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log-odds

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Recall that: k is the number of β 's (here p + 1)

Odds:

$$\frac{Pr(Y=1|\mathbf{X}=\mathbf{x})}{Pr(Y=0|\mathbf{X}=\mathbf{x})} = e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}$$

Let's call
$$\pi_1 = Pr(Y=1|\mathbf{X}=\mathbf{x}_1)$$

$$\pi_2 = Pr(Y=1|\mathbf{X}=\mathbf{x}_2)$$

Then :

$$odds_1 = \frac{\pi_1}{(1 - \pi_1)}$$
 and $odds_2 = \frac{\pi_2}{(1 - \pi_2)}$

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Let's call
$$\pi_1 = Pr(Y = 1 | \mathbf{X} = \mathbf{x}_1) \xrightarrow{\text{Examples:}}_{\substack{\text{Non-Smoking} \\ \text{vs.} \\ \text{vs.} \\ \text{Smoking} \\ \text{Treatment}}}$$

$$\pi_2 = Pr(Y = 1 | \mathbf{X} = \mathbf{x}_2)$$

Then :

$$odds_1 = \frac{\pi_1}{(1 - \pi_1)}$$
 and $odds_2 = \frac{\pi_2}{(1 - \pi_2)}$

probability

$$\pi_1 = Pr(Y = 1 | \mathbf{X} = \mathbf{x}_1)$$
 and $\pi_2 = Pr(Y = 1 | \mathbf{X} = \mathbf{x}_2)$

odds

$$odds_1 = \frac{\pi_1}{(1 - \pi_1)}$$
 and $odds_2 = \frac{\pi_2}{(1 - \pi_2)}$

Odds Ratio

$$OR = \frac{\frac{\pi_1}{(1 - \pi_1)}}{\frac{\pi_2}{(1 - \pi_2)}}$$





Disease



X=1



ODDS RATIO (5/3) / (3/5) = 25/9 = 2.778

The odds of being diseased are 2.778 times higher for smokers than for non-smokers.

Interpretation:



smokers than for non-smokers.





Disease

Y = 1

Y = 0

Sex

Male $X_2 = 0$

X₂ = 1

Female

X₁=1



odds

Sex Male $X_2 = 0$ Female 🔲 $X_2 = 1$

Disease

Y = 1 🚫

Y = 0



odds ratio

odds

OR_{male}: 3:1

OR_{female}: 3:1



odds ratio

odds

OR_{male}: 3:1

OR_{female}: 3:1

.... so do we have OR = 3 or OR = 2.778 ?



Notes:

- This has nothing to do with unobserved confounding, same thing happens if we randomize subjects.
 (Exercise : Check to see that cor(x₁, x₂) = 0)
- This happens because of the "non-collapsibility" of the OR.

Reading : "Second argument: Omitted non-confounders in logistic regression" http://jakewestfall.org/blog/index.php/2018/03/12/logistic-regression-is-not-fucked/



In both these example the covariate "X" is uncorrelated with the covariate "Colour"

Yet, since the logistic function is not collapsible, the average of the blue and red curves is not equal to the black curve.... very curious...

- Maybe there are better measure to describe the effect?
- Since OR is so difficult to interpret, perhaps we should use RR?

Expression	Domain	Null Value	
$\pi_1 - \pi_2$	[-1, 1]	0	
π_1/π_2	$(0,\infty)$	1	
$\log(\pi_1) - \log\left(\pi_2\right)$	$(-\infty,\infty)$	0	
$rac{\pi_1/(1-\pi_1)}{\pi_2/(1-\pi_2)}$	$(0,\infty)$	1	
$\log \frac{\pi_1}{1 - \pi_1} - \log \frac{\pi_2}{1 - \pi_2}$	$(-\infty,\infty)$	0	
	$Expression \pi_1 - \pi_2 \pi_1/\pi_2 \log(\pi_1) - \log(\pi_2) \frac{\pi_1/(1 - \pi_1)}{\pi_2/(1 - \pi_2)} \log\frac{\pi_1}{1 - \pi_1} - \log\frac{\pi_2}{1 - \pi_2}$	Expression Domain $\pi_1 - \pi_2$ $[-1, 1]$ π_1/π_2 $(0, \infty)$ $\log(\pi_1) - \log(\pi_2)$ $(-\infty, \infty)$ $\frac{\pi_1/(1 - \pi_1)}{\pi_2/(1 - \pi_2)}$ $(0, \infty)$ $\log \frac{\pi_1}{1 - \pi_1} - \log \frac{\pi_2}{1 - \pi_2}$ $(-\infty, \infty)$	

Biostatistical Methods: The Assessment of Relative Risks By John M. Lachin To convert an Odds Ratio to a Relative Risk, you need to know π_1 , which in our example is Pr(Y=1|X=0). Here is the formula:

$$RR = OR/(1 - \pi_1 + (\pi_1 \cdot OR))$$

(Exercise : Derive the formula.)



More info: http://www.bmj.com/content/bmj/348/bmj.f7450.full.pdf



	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0	0.59	0.33	0.17	0.08	0.03	0.01	0.00	0.00	0.00
1	0.33	0.41	0.36	0.26	0.16	0.08	0.03	0.01	0.00
2	0.07	0.20	0.31	0.35	0.31	0.23	0.13	0.05	0.01
3	0.01	0.05	0.13	0.23	0.31	0.35	0.31	0.20	0.07
4	0.00	0.01	0.03	0.08	0.16	0.26	0.36	0.41	0.33
5	0.00	0.00	0.00	0.01	0.03	0.08	0.17	0.33	0.59

$$Prob(\pi|N,k) = \binom{N}{k} \cdot \pi^k (1-k)^{N-k}$$



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5	0.00	0.00	0.00	0.01	0.03	0.08	0.17	0.33	0.59

Examples:

Prob($\pi = 0.5 \mid 0$ heads out of 5 tosses) = 0.03

Prob(π = 0.2 | 4 heads out of 5 tosses) = 0.01





number_heads

2

5

Out of 5 tosses







Out of 10 tosses

















Out of 5 tosses









Disease



5/8

X=1



5/8

smokers



 π_1



smokers

5/8

X=0

X=1



General definition of likelihood

Let data (y_1, \ldots, y_n) be realization of a random vector (Y_1, \ldots, Y_n) with density or model $f_{Y_1, \ldots, Y_n}(y_1, \ldots, y_n; \theta)$ where θ is the parameter (usually a vector). The parameter θ is unknown and the best "guess" is estimated from the data (y_1, \ldots, y_n) by maximizing (over θ) the function:

$$L(oldsymbol{ heta}; ext{data}) = f_{Y_1,...,Y_n}(y_1,\ldots,y_n;oldsymbol{ heta}).$$

After data are observed, consider (y_1, \ldots, y_n) as fixed and $\boldsymbol{\theta}$ as a quantity to be estimated. The parameter value $\boldsymbol{\theta}_1$ is more consistent with the data than $\boldsymbol{\theta}_2$ if

$$L(oldsymbol{ heta}_1; ext{data}) = f_{Y_1,\dots,Y_n}(y_1,\dots,y_n;oldsymbol{ heta}_1) > f_{Y_1,\dots,Y_n}(y_1,\dots,y_n;oldsymbol{ heta}_2) = L(oldsymbol{ heta}_2; ext{data})$$

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If Y_1, \ldots, Y_n are independent random variables, then the joint density is a product of univariate densities

$$f_{Y_1,...,Y_n}(y_1,\ldots,y_n;oldsymbol{ heta}) = \prod_{i=1}^n f_{Y_i}(y_i;oldsymbol{ heta})$$

The maximum likelihood estimate $\hat{\boldsymbol{\theta}}$ maximizes $L(\boldsymbol{\theta}; \text{data})$ in (6.11), or equivalently maximizes $\log L(\boldsymbol{\theta}; \text{data})$ and minimizes $-\log L(\boldsymbol{\theta}; \text{data})$.

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(6.13)
$$f_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n;\theta) = \prod_{i=1}^n f_{Y_i}(y_i;\theta).$$

Coin toss example:
$$\int_{0}^{0} \int_{0}^{0} \int$$

If there are explanatory variables (considered as non-random), and response variables are considered as realizations of random variables, then the likelihood is:

(6.14)
$$L(\boldsymbol{\theta}; \text{data}) = f_{Y_1, \dots, Y_n}(y_1, \dots, y_n; \boldsymbol{\theta}, \text{explanatory } \mathbf{x}_1, \dots, \mathbf{x}_n).$$

This can get difficult to work with, since it involves lots of multiplications...

So instead we often work with the log-likelihood, log(L).

Consider only sample of Y ... what is the maximum likelihood estimate for mu?



 $logLikelihood(\mu|y) = -\frac{1}{2}n\log(2\pi) - \frac{1}{2}n\log(\sigma^2) - \frac{1}{2}\sum_{i=1}^{n}(y_i - \mu)^2/(2\sigma^2)$

Example 6.6 Gaussian regression and homoscedasticity assumption.

 $Y_i \sim N(\mu_i = \mathbf{x}_i^T \boldsymbol{\beta}, \sigma^2)$, independently with $\mathbf{x}_i^T = (1, x_{i1}, \dots, x_{ip})$. Here $\boldsymbol{\theta} = (\boldsymbol{\beta}, \sigma^2)$ and $\boldsymbol{\beta}^T = (\beta_0, \beta_1, \dots, \beta_p)$. The likelihood and log-likelihood are:

(6.15)
$$L(\boldsymbol{\theta}; \text{data}) = \prod_{i=1}^{n} f_{Y_i}(y_i; \mu_i, \sigma^2) = \prod_{i=1}^{n} \frac{1}{(2\pi)^{1/2} \sigma} \exp\{-\frac{1}{2} (y_i - \mu_i)^2 / \sigma^2\}$$

(6.16)
$$= \frac{1}{(2\pi)^{n/2}\sigma^n} \exp\left\{-\frac{1}{2}\sum_{i=1}^n (y_i - \mu_i)^2 / \sigma^2\right\},$$

(6.17)
$$\log L(\boldsymbol{\theta}; \text{data}) = -\frac{1}{2}n\log(2\pi) - n\log\sigma - \frac{1}{2}\sum_{i=1}^{n}(y_i - \mu_i)^2/\sigma^2$$

(6.18)
$$= -\frac{1}{2}n\log(2\pi) - \frac{1}{2}n\log\sigma^2 - \frac{1}{2}\sum_{i=1}^n (y_i - \mathbf{x}_i^T\boldsymbol{\beta})^2/\sigma^2.$$

For any fixed σ^2 , maximizing the likelihood is the same as maximizing the log-likelihood, or minimizing $\sum_{i=1}^{n} (y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2$ (that is, least squares). Next, if the parameter σ^2 is also optimized in the likelihood, then its maximum likelihood estimate is $\sum_i e_i^2/n$ instead of $\hat{\sigma}^2 = \sum_i e_i^2/(n-k)$, where e_i are the residuals from least squares. [Check as an exercise].

Now consider Y and X ... what is the maximum likelihood estimate for β ?



 β_1

 $\operatorname{Cov}(\hat{\boldsymbol{\theta}})$. Let $\hat{\boldsymbol{\theta}}$ be the maximum likelihood estimate.

Equation for (asymptotic) standard errors, square root of the diagonal of the inverse of the negative Hessian matrix:

$$\left[-rac{\partial^2 \log L(oldsymbol{ heta}; ext{data})}{\partial oldsymbol{ heta} \partial oldsymbol{ heta}^T} \left|_{oldsymbol{ heta}}
ight|_{oldsymbol{ heta}}
ight|_{oldsymbol{ heta}}
ight]^{-1},$$

that is, get the Hessian matrix of negative second order derivatives, take the inverse, extract the diagonal components and take square roots.

The Hessian of g measures the curvature of the negative log-likelihood surface at $\hat{\theta}$. The sharper the curvature is, the smaller the "uncertainty" and the smaller \pm figure for the SE.

The more curved the surface (or parabola if θ has dimension 1), the larger the Hessian (second derivative)

and the smaller the inverse Hessian. SEs come from the sqrt of the diagonal elements of the inverse Hessian.

 $\operatorname{Cov}(\hat{\boldsymbol{\theta}})$. Let $\hat{\boldsymbol{\theta}}$ be the maximum likelihood estimate.

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that is, get the Hessian matrix of negative second order derivatives, take the inverse, extract the diagonal components and take square roots.

Check what this becomes for the log-likelihood for $Y_i \sim N(\mu_i, \sigma^2)$.

$$\begin{aligned} -\log L(\boldsymbol{\theta}; \text{data}) &= \frac{1}{2}n\log(2\pi) + n\log\sigma + \frac{1}{2}\sum_{i=1}^{n}(y_{i} - \mathbf{x}_{i}^{T}\boldsymbol{\beta})^{2}/\sigma^{2} \\ &= \frac{1}{2}n\log(2\pi) + n\log\sigma + \frac{1}{2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^{T}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})/\sigma^{2} \\ -\frac{\partial\log L(\boldsymbol{\theta}; \text{data})}{\partial \boldsymbol{\beta}} &= -\frac{\mathbf{X}^{T}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}{\sigma^{2}} \\ -\frac{\partial^{2}\log L(\boldsymbol{\theta}; \text{data})}{\partial \boldsymbol{\beta}\partial \boldsymbol{\beta}^{T}} &= \frac{\mathbf{X}^{T}\mathbf{X}}{\sigma^{2}} \end{aligned}$$

Inverse is $\sigma^2 (\mathbf{X}^T \mathbf{X})^{-1}$. For standard errors, substitute $\hat{\sigma}$ for σ , and get square root of diagonal elements. The above uses matrix/vector derivatives — Section 3.2.

The log-likelihood for logistic regression:

$$\log L(\boldsymbol{\beta}; \text{data}) = \sum_{i=1}^{n} (\mathbf{x}_{i}^{T} \boldsymbol{\beta}) y_{i} - \sum_{i=1}^{n} \log[1 + \exp\{\mathbf{x}_{i}^{T} \boldsymbol{\beta}\}]$$

and the

logistic negative log-likelihood

$$-\log L(oldsymbol{eta}; ext{data}) = -\sum_{i=1}^n (\mathbf{x}_i^Toldsymbol{eta})y_i + \sum_{i=1}^n \log[1+\exp\{\mathbf{x}_i^Toldsymbol{eta}\}]$$

Unfortunately...

There is no closed form solution, but statistical software obtain $\hat{\beta}_0, \hat{\beta}_1$ with an iterative method.

To get standard errors, confidence intervals, we must get the second derivative of **the logistic negative log-likelihood**:

Let $\pi_i = \pi_i(\mathbf{x}_i; \boldsymbol{\beta}) = \exp\{\mathbf{x}_i^T \boldsymbol{\beta}\}/[1 + \exp\{\mathbf{x}_i^T \boldsymbol{\beta}\}] = 1/[1 + \exp\{-\mathbf{x}_i^T \boldsymbol{\beta}\}], 1 - \pi_i = 1/[1 + \exp\{\mathbf{x}_i^T \boldsymbol{\beta}\}].$ The gradient

vector is:

$$-\frac{\partial \log L(\boldsymbol{\beta}; \text{data})}{\partial \boldsymbol{\beta}} = -\sum_{i=1}^{n} \mathbf{x}_{i} y_{i} + \sum_{i=1}^{n} \mathbf{x}_{i} \frac{\exp\{\mathbf{x}_{i}^{T} \boldsymbol{\beta}\}}{1 + \exp\{\mathbf{x}_{i}^{T} \boldsymbol{\beta}\}} = -\sum_{i=1}^{n} \mathbf{x}_{i} y_{i} + \sum_{i=1}^{n} \mathbf{x}_{i} \pi_{i}$$

The Hessian matrix of second order derivatives is:

$$-\frac{\partial^2 \log L(\boldsymbol{\beta}; \text{data})}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^T} = \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^T \pi_i (1 - \pi_i), \tag{1}$$

making use of $\frac{d}{dz}\frac{z}{1+z} = \frac{1}{(1+z)^2}$ and $dz/d\boldsymbol{\beta}^T = \mathbf{x}^T z, \ z = \exp\{\mathbf{x}^T \boldsymbol{\beta}\}.$

When (1) is evaluated at the maximum likelihood estimate, π_i is replaced by $\hat{\pi}_i = 1/[1 + \exp\{-\mathbf{x}_i^T \hat{\boldsymbol{\beta}}\}]$. To check that this is valid, try to get this result in non-matrix form when p = 1 (one explanatory variable).

Summary

concept $response type$	continuous/normal	binary
linearity	$\mid \mu_i = \mathbf{x}_i^T \boldsymbol{eta}$	$\log rac{\pi_i}{1-\pi_i} = \mathbf{x}_i^T oldsymbol{eta}$
no \mathbf{x} effect	$SS(Total) = \sum (y_i - \overline{y})^2$	nulldev= $-2[y_+ \log(\frac{y_+}{n}) + (n - y_+) \log(1 - \frac{y_+}{n})]$
\mathbf{x} effect	$SS(Res; \mathbf{x}) = \sum (y_i - \hat{y}_i)^2$	residdev=-2loglik at MLE
$\operatorname{Cov}(\hat{\boldsymbol{\beta}})$	$\hat{\sigma}^2 [\sum_i \mathbf{x}_i \mathbf{x}_i^T]^{-1}$	$[\sum_i \hat{\pi}_i (1 - \hat{\pi}_i) \mathbf{x}_i \mathbf{x}_i^T]^{-1}$
variability explained	R^2 , adj R^2	none
$- loglik \left[\mathbf{X}_{subset} \right]$	C_p	AIC = -2(loglik-#parameters)
out-of-sample pred	CVRMSE	out-of-sample misclassification
in-sample	σ	in-sample misclassification

In the above $y_+ = \sum_{i=1}^n y_i$ and the sample proportion is y_+/n .

For AIC=Akaike information criterion, smaller is better.

$$C_p = \frac{SS(Res;subset)}{MS(Res;full)} + 2 \times ncol(\mathbf{X}_{subset}) - n; \ \# parameters = ncol(\mathbf{X}_{subset}), \ ignoring \ \sigma^2$$