## 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:

$$
\begin{gathered}
\log \left(\frac{\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x}}{\operatorname{Pr}(Y=0 \mid \mathbf{X}=\mathbf{x}}\right)=\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p} \\
\frac{\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x})}{\operatorname{Pr}(Y=0 \mid \mathbf{X}=\mathbf{x})}=e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}} \\
\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x})=\frac{e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}}}{1+e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}}}
\end{gathered}
$$

From last lecture, we have three equivalent ways to write out the logistic regression model:
log-odds
$\log \left(\frac{\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x}}{\operatorname{Pr}(Y=0 \mid \mathbf{X}=\mathbf{x}}\right)=\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}$

$$
\begin{gathered}
\frac{\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x})}{\operatorname{Pr}(Y=0 \mid \mathbf{X}=\mathbf{x})}=e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}} \\
\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x})=\frac{e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}}}{1+e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}}}
\end{gathered}
$$

## Odds:

$$
\frac{\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x})}{\operatorname{Pr}(Y=0 \mid \mathbf{X}=\mathbf{x})}=e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}}
$$

Let's call

$$
\begin{aligned}
& \pi_{1}=\operatorname{Pr}\left(Y=1 \mid \mathbf{X}=\mathbf{x}_{1}\right) \\
& \pi_{2}=\operatorname{Pr}\left(Y=1 \mid \mathbf{X}=\mathbf{x}_{2}\right)
\end{aligned}
$$

Then :

$$
o d d s_{1}=\frac{\pi_{1}}{\left(1-\pi_{1}\right)} \quad \text { and } \quad o d d s_{2}=\frac{\pi_{2}}{\left(1-\pi_{2}\right)}
$$

## Odds:

$$
\frac{\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x})}{\operatorname{Pr}(Y=0 \mid \mathbf{X}=\mathbf{x})}=e^{\beta_{0}+\beta_{1} x_{1}+\ldots+\beta_{p} x_{p}}
$$

Let's call

$$
\begin{aligned}
& \pi_{1}=\operatorname{Pr}\left(Y=1 \mid \mathbf{X}=\mathbf{x}_{1}\right){ }_{\substack{\text { Placebo } \\
\text { vs. } \\
\text { vxamples: } \\
\text { Treatment }}}^{\text {vs. }} \\
& \pi_{2}=\operatorname{Pr}\left(Y=1 \mid \mathbf{X}=\mathbf{x}_{2}\right)
\end{aligned}
$$

Non-Smoking
Smoking

Then :

$$
\text { odds }_{1}=\frac{\pi_{1}}{\left(1-\pi_{1}\right)} \quad \text { and } \quad o d d s_{2}=\frac{\pi_{2}}{\left(1-\pi_{2}\right)}
$$

probability

$$
\pi_{1}=\operatorname{Pr}\left(Y=1 \mid \mathbf{X}=\mathbf{x}_{1}\right) \quad \text { and } \quad \pi_{2}=\operatorname{Pr}\left(Y=1 \mid \mathbf{X}=\mathbf{x}_{2}\right)
$$

odds

$$
o d d s_{1}=\frac{\pi_{1}}{\left(1-\pi_{1}\right)} \quad \text { and } \quad o d d s_{2}=\frac{\pi_{2}}{\left(1-\pi_{2}\right)}
$$

Odds Ratio

$$
O R=\frac{\frac{\pi_{1}}{\left(1-\pi_{1}\right)}}{\frac{\pi_{2}}{\left(1-\pi_{2}\right)}}
$$



Disease

$$
\begin{aligned}
& \mathrm{Y}=1 \\
& \mathrm{Y}=0
\end{aligned}
$$


smokers
$X=1$

probability
odds
odds $_{x=0}=3 / 5=0.6$

$$
\operatorname{Pr}(\mathrm{Y}=1 \mid \mathrm{X}=0)=5 / 8=0.625
$$

$$
\text { odds }_{x=1}=5 / 3=1.667
$$

## ODDS RATIO <br> $$
(5 / 3) /(3 / 5)=25 / 9=2.778
$$

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

$$
\operatorname{Pr}(Y=1 \mid X=0)=3 / 8=0.375
$$

$$
\operatorname{odds}_{x=0}=3 / 5=0.6
$$

non-smokers
$X=0$

## Disease

$$
\begin{aligned}
& Y=1 \\
& Y=0
\end{aligned}
$$


$X=1$

$$
\begin{aligned}
& \operatorname{Pr}(\mathrm{Y}=1 \mid \mathrm{X}=0)=5 / 8=0.625 \\
& \text { odds }_{\mathrm{X}=1}=5 / 3=1.667
\end{aligned}
$$

probability
odds
Exercise: Recall the logistic model: $\quad \log \left(\frac{\operatorname{Pr}(Y=1 \mid \mathbf{X}=\mathbf{x}}{\operatorname{Pr}(Y=0 \mid \mathbf{X}=\mathbf{x}}\right)=\beta_{0}+\beta_{1} x_{1} \quad \ldots$. Therefore: $\quad \mathrm{OR}=\exp \left(\beta_{1}\right)$

$$
(5 / 3) /(3 / 5)=25 / 9=2.778
$$

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



odds ratio

$$
\mathrm{OR}_{\text {male }}: 3: 1
$$

$$
\mathrm{OR}_{\text {female }}: 3: 1
$$



Disease

$$
\begin{aligned}
& Y=1 \\
& Y=0
\end{aligned}
$$

## Sex

## Male

 $\mathrm{X}_{2}=0$$$
X_{1}=1
$$

$$
\operatorname{Pr}\left(Y=1 \mid X_{1}=1, X_{2}=0\right)=3 / 4=0.75
$$

$$
\operatorname{Pr}\left(Y=1 \mid X_{1}=1, X_{2}=1\right)=2 / 4=0.5
$$

$$
\text { odds }_{x 1=1, x 2=0}=3 / 1=3
$$

$$
\operatorname{odds}_{x 1=1, x 2=1}=2 / 2=1
$$

probability

$$
\begin{aligned}
& \operatorname{Pr}\left(Y=1 \mid X_{1}=0, X_{2}=0\right)=2 / 4=0.5 \\
& \operatorname{Pr}\left(Y=1 \mid X_{1}=0, X_{2}=1\right)=1 / 4=0.25
\end{aligned}
$$

odds

$$
\begin{aligned}
& \text { odds }_{x 1=0, x_{2}=0}=2 / 2=1: 1 \\
& \text { odds }_{x 1=0, x_{2}=1}=1 / 3=0.333
\end{aligned}
$$


odds ratio

$$
\mathrm{OR}_{\text {male }}: 3: 1 \quad \mathrm{OR}_{\text {female }}: 3: 1
$$

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?

| Type $\theta$ | Expression | Domain | Null Value |
| :---: | :---: | :---: | :---: |
| Risk difference $(R D)$ | $\pi_{1}-\pi_{2}$ | $[-1,1]$ | 0 |
| Relative risk $(R R)$ | $\pi_{1} / \pi_{2}$ | $(0, \infty)$ | 1 |
| $\log R R$ | $\log \left(\pi_{1}\right)-\log \left(\pi_{2}\right)$ | $(-\infty, \infty)$ | 0 |
| Odds ratio (OR) | $\frac{\pi_{1} /\left(1-\pi_{1}\right)}{\pi_{2} /\left(1-\pi_{2}\right)}$ | $(0, \infty)$ | 1 |
| $\log$ OR | $\log \frac{\pi_{1}}{1-\pi_{1}}-\log \frac{\pi_{2}}{1-\pi_{2}}$ | $(-\infty, \infty)$ | 0 |

Biostatistical Methods: The Assessment of Relative Risks By John M. Lachin

To convert an Odds Ratio to a Relative Risk, you need to know $\pi_{1}$, which in our example is $\operatorname{Pr}(\mathrm{Y}=1 \mid \mathrm{X}=0)$. Here is the formula:

$$
R R=O R /\left(1-\pi_{1}+\left(\pi_{1} \cdot O R\right)\right)
$$

(Exercise : Derive the formula.)


## Maximum Likelihood with 5 coins tosses...

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

## Maximum Likelihood with 5 coins tosses...

|  | 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 |

Examples:

$$
\begin{aligned}
& \operatorname{Prob}(\pi=0.5 \mid 0 \text { heads out of } 5 \text { tosses })=0.03 \\
& \operatorname{Prob}(\pi=0.2 \mid 4 \text { heads out of } 5 \text { tosses })=0.01
\end{aligned}
$$

## Maximum Likelihood with 5 coins tosses...


number_heads
$\rightarrow 0$
$\rightarrow 1$
$\rightarrow 2$
$-3$
$-4$
$\rightarrow-5$

## Maximum Likelihood with 5 coins tosses...



## Maximum Likelihood with 5 coins tosses...



## Maximum Likelihood with 5 coins tosses...



## Maximum Likelihood with 5 coins tosses...


number_heads

## Maximum Likelihood with 5 coins tosses...



Out of 5 tosses

$3 / 8$
non-smokers

## 5/8

smokers

$3 / 8$
non-smokers
$X=0$

## 5/8

smokers
$X=1$


General definition of likelihood
Let data $\left(y_{1}, \ldots, y_{n}\right)$ be realization of a random vector $\left(Y_{1}, \ldots, Y_{n}\right)$ with density or model $f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}\right)$ where $\boldsymbol{\theta}$ is the parameter (usually a vector). The parameter $\boldsymbol{\theta}$ is unknown and the best "guess" is estimated from the data $\left(y_{1}, \ldots, y_{n}\right)$ by maximizing (over $\boldsymbol{\theta}$ ) the function:

$$
L(\boldsymbol{\theta} ; \text { data })=f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}\right)
$$

After data are observed, consider $\left(y_{1}, \ldots, y_{n}\right)$ 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

$$
L\left(\boldsymbol{\theta}_{1} ; \text { data }\right)=f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}_{1}\right)>f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}_{2}\right)=L\left(\boldsymbol{\theta}_{2} ; \text { data }\right) .
$$

General definition of likelihood
Let data $\left(y_{1}, \ldots, y_{n}\right)$ be realization of a random vector $\left(Y_{1}, \ldots, Y_{n}\right)$ with density or model $f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}\right)$ where $\boldsymbol{\theta}$ is the parameter (usually a vector). The parameter $\boldsymbol{\theta}$ is unknown and the best "guess" is estimated from the data $\left(y_{1}, \ldots, y_{n}\right)$ by maximizing (over $\left.\boldsymbol{\theta}\right)$ the function:

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$$
L\left(\boldsymbol{\theta}_{1} ; \text { data }\right)=f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}_{1}\right)>f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}_{2}\right)=L\left(\boldsymbol{\theta}_{2} ; \text { data }\right) .
$$

If $Y_{1}, \ldots, Y_{n}$ are independent random variables, then the joint density is a product of univariate densities

$$
f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}\right)=\prod_{i=1}^{n} f_{Y_{i}}\left(y_{i} ; \boldsymbol{\theta}\right)
$$

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

If $Y_{1}, \ldots, Y_{n}$ are independent random variables, then the joint density is a product of univariate densities

$$
\begin{equation*}
f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}\right)=\prod_{i=1}^{n} f_{Y_{i}}\left(y_{i} ; \boldsymbol{\theta}\right) . \tag{6.13}
\end{equation*}
$$

Coin toss example:


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

$$
\begin{equation*}
L(\boldsymbol{\theta} ; \text { data })=f_{Y_{1}, \ldots, Y_{n}}\left(y_{1}, \ldots, y_{n} ; \boldsymbol{\theta}, \text { explanatory } \mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right) . \tag{6.14}
\end{equation*}
$$

This can get difficult to work with, since it involves lots of multiplications...
So instead we often work with the $\log$-likelihood, $\log (\mathrm{L})$.

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


Likelihood $(\mu \mid y)=\prod_{i=1}^{n} \frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(\left(y_{i}-\mu\right)^{2} /\left(2 \sigma^{2}\right)\right.$

Sample, $n=9$
并
$\log L i k e l i h o o d(\mu \mid y)=-\frac{1}{2} n \log (2 \pi)-\frac{1}{2} n \log \left(\sigma^{2}\right)-\frac{1}{2} \sum_{i=1}^{n}\left(y_{i}-\mu\right)^{2} /\left(2 \sigma^{2}\right)$

## Example 6.6 Gaussian regression and homoscedasticity assumption.

$Y_{i} \sim N\left(\mu_{i}=\mathbf{x}_{i}^{T} \boldsymbol{\beta}, \sigma^{2}\right)$, independently with $\mathbf{x}_{i}^{T}=\left(1, x_{i 1}, \ldots, x_{i p}\right)$. Here $\boldsymbol{\theta}=\left(\boldsymbol{\beta}, \sigma^{2}\right)$ and $\boldsymbol{\beta}^{T}=$ $\left(\beta_{0}, \beta_{1}, \ldots, \beta_{p}\right)$. The likelihood and $\log$-likelihood are:

$$
\begin{align*}
L(\boldsymbol{\theta} ; \text { data }) & =\prod_{i=1}^{n} f_{Y_{i}}\left(y_{i} ; \mu_{i}, \sigma^{2}\right)=\prod_{i=1}^{n} \frac{1}{(2 \pi)^{1 / 2} \sigma} \exp \left\{-\frac{1}{2}\left(y_{i}-\mu_{i}\right)^{2} / \sigma^{2}\right\}  \tag{6.15}\\
& =\frac{1}{(2 \pi)^{n / 2} \sigma^{n}} \exp \left\{-\frac{1}{2} \sum_{i=1}^{n}\left(y_{i}-\mu_{i}\right)^{2} / \sigma^{2}\right\},  \tag{6.16}\\
\log L(\boldsymbol{\theta} ; \text { data }) & =-\frac{1}{2} n \log (2 \pi)-n \log \sigma-\frac{1}{2} \sum_{i=1}^{n}\left(y_{i}-\mu_{i}\right)^{2} / \sigma^{2}  \tag{6.17}\\
& =-\frac{1}{2} n \log (2 \pi)-\frac{1}{2} n \log \sigma^{2}-\frac{1}{2} \sum_{i=1}^{n}\left(y_{i}-\mathbf{x}_{i}^{T} \boldsymbol{\beta}\right)^{2} / \sigma^{2} . \tag{6.18}
\end{align*}
$$

For any fixed $\sigma^{2}$, maximizing the likelihood is the same as maximizing the log-likelihood, or minimizing $\sum_{i=1}^{n}\left(y_{i}-\right.$ $\left.\mathbf{x}_{i}^{T} \boldsymbol{\beta}\right)^{2}$ (that is, least squares). Next, if the parameter $\sigma^{2}$ 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 $X \ldots$ what is the maximum likelihood estimate for $\boldsymbol{\beta}$ ?

$\operatorname{Likelihood}(\beta \mid y, X)=\prod_{i=1}^{n} \frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(\left(y_{i}-X^{T} \beta\right)^{2} /\left(2 \sigma^{2}\right)\right.$
$\log \operatorname{Likelihood}(\beta \mid y, X)=-\frac{1}{2} n \log (2 \pi)-\frac{1}{2} n \log \left(\sigma^{2}\right)-\frac{1}{2} \sum_{i=1}^{n}\left(y_{i}-X^{T} \beta\right)^{2} /\left(2 \sigma^{2}\right)$
$\operatorname{Cov}(\hat{\boldsymbol{\theta}})$. 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:

$$
\left[-\left.\frac{\partial^{2} \log L(\boldsymbol{\theta} ; \text { data })}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^{T}}\right|_{\hat{\boldsymbol{\theta}}}\right]^{-1}
$$

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 sürface at $\hat{\boldsymbol{\theta}}$. 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 $\boldsymbol{\theta}$ 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.
Equation for (asymptotic) standard errors, square root of the diagonal of the inverse of the negative Hessian matrix:

$$
\left[-\left.\frac{\partial^{2} \log L(\boldsymbol{\theta} ; \text { data })}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^{T}}\right|_{\hat{\boldsymbol{\theta}}}\right]^{-1},
$$

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 $Y_{i} \sim N\left(\mu_{i}, \sigma^{2}\right)$.

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

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

The log-likelihood for logistic regression:

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

and the
logistic negative log-likelihood

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

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 $\pi_{i}=\pi_{i}\left(\mathbf{x}_{i} ; \boldsymbol{\beta}\right)=\exp \left\{\mathbf{x}_{i}^{T} \boldsymbol{\beta}\right\} /\left[1+\exp \left\{\mathbf{x}_{i}^{T} \boldsymbol{\beta}\right\}\right]=1 /\left[1+\exp \left\{-\mathbf{x}_{i}^{T} \boldsymbol{\beta}\right\}\right], 1-\pi_{i}=1 /\left[1+\exp \left\{\mathbf{x}_{i}^{T} \boldsymbol{\beta}\right\}\right]$. The gradient vector is:

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

The Hessian matrix of second order derivatives is:

$$
\begin{equation*}
-\frac{\partial^{2} \log L(\boldsymbol{\beta} ; \text { data })}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^{T}}=\sum_{i=1}^{n} \mathbf{x}_{i} \mathbf{x}_{i}^{T} \pi_{i}\left(1-\pi_{i}\right), \tag{1}
\end{equation*}
$$

making use of $\frac{d}{d z} \frac{z}{1+z}=\frac{1}{(1+z)^{2}}$ and $d z / d \boldsymbol{\beta}^{T}=\mathbf{x}^{T} z, z=\exp \left\{\mathbf{x}^{T} \boldsymbol{\beta}\right\}$.
When (1) is evaluated at the maximum likelihood estimate, $\pi_{i}$ is replaced by $\hat{\pi}_{i}=1 /\left[1+\exp \left\{-\mathbf{x}_{i}^{T} \hat{\boldsymbol{\beta}}\right\}\right]$. To check
that this is valid, try to get this result in non-matrix form when $p=1$ (one explanatory variable).

Summary

| concept $\backslash$ response type | continuous/normal | binary |
| :--- | :--- | :--- |
| linearity | $\mu_{i}=\mathbf{x}_{i}^{T} \boldsymbol{\beta}$ | $\log \frac{\pi_{i}}{1-\pi_{i}}=\mathbf{x}_{i}^{T} \boldsymbol{\beta}$ |
| no $\mathbf{x}$ effect | $S S($ Total $)=\sum\left(y_{i}-\bar{y}\right)^{2}$ | nulldev $=-2\left[y_{+} \log \left(\frac{y_{+}}{n}\right)+\left(n-y_{+}\right) \log \left(1-\frac{y_{+}}{n}\right)\right]$ |
| $\mathbf{x}$ effect | $S S(\operatorname{Res} ; \mathbf{x})=\sum\left(y_{i}-\hat{y}_{i}\right)^{2}$ | residdev $=-2 \log l i k$ at MLE |
| Cov $(\hat{\boldsymbol{\beta}})$ | $\hat{\sigma}^{2}\left[\sum_{i} \mathbf{x}_{i} \mathbf{x}^{T}\right]^{-1}$ | $\left[\sum_{i} \hat{\pi}_{i}\left(1-\hat{\pi}_{i}\right) \mathbf{x}_{i} \mathbf{x}_{i}^{T}\right]^{-1}$ |
| variability explained | $R^{2}$, adj $R^{2}$ | none |
| -loglik $\left[\mathbf{X}_{\text {subset }}\right]$ | $C_{p}$ | AIC $=-2(\operatorname{loglik-\# parameters)~}$ |
| out-of-sample pred | CVRMSE | out-of-sample misclassification |
| in-sample | $\hat{\sigma}$ | 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.
$C_{p}=\frac{S S(\text { Res;subset })}{M S(\text { Res:full })}+2 \times \operatorname{ncol}\left(\mathbf{X}_{\text {subset }}\right)-n ; \#$ parameters $=\operatorname{ncol}\left(\mathbf{X}_{\text {subset }}\right)$, ignoring $\sigma^{2}$

