# STOR 556: ADV METH DATA ANAL Instructor: Richard L. Smith 

Class Notes \#7:
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THE UNIVERSITY<br>of NORTH CAROLINA<br>at CHAPEL HILL

## Homework 3: Due Tuesday, February 5

Questions 2 and 3 of the problems on pages 47/48

- Submit through sakai "Assignments" tab
- Repeated submissions are permitted but not encouraged
- Deadline will be 11:55 pm, Tuesday February 5
- pdf file preferred
- I suggest you name the file something similar to "Richard_Smith_HW3.pdf" (substituting your own name of course). This will help the grader keep track of the submissions.


## Scheduling a Take-home Midterm/Final

- Midterm, posted noon Feb 24, email solutions no later than 6pm Feb 25
- Final, posted noon Apr 30, email solutions no later than 6pm May 1
- I'd now like to make these dates definite but will work with any individual students who have difficulties with those dates


## LOGISTIC REGRESSION

- $y_{i}$ is 0 or 1 , covariates $x_{i j}, 0 \leq j \leq p, 1 \leq i \leq n$.
- Define $p_{i}=\operatorname{Pr}\left\{y_{i}=1 \mid x_{i 0}, \ldots, x_{i p}\right\}$.
- $p_{i}=\sum_{j=0}^{p} x_{i j} \beta_{j}$ makes no sense
- Instead, define $\operatorname{logit}(p)=\log \left(\frac{p}{1-p}\right)$.
- $\operatorname{logit}\left(p_{i}\right)=\sum_{j=0}^{p} x_{i j} \beta_{j}$ or $p_{i}=\frac{\exp \left(\sum_{j=0}^{p} x_{i j} \beta_{j}\right)}{1+\exp \left(\sum_{j=0}^{p} x_{i j} \beta_{j}\right)}$.
- Fit in R by a command of form glmod=glm(y~x1+x2,family=binomial) with any number of covariates in the sum.


## METHOD OF MAXIMUM LIKELIHOOD

- $Y_{1}, \ldots, Y_{n}$ are observations, independent.
- Density of $Y_{i}$ is $f_{i}(\cdot ; \theta)$ where $\theta$ is a vector of parameters
- Density may refer to discrete case (probability mass function), continuous case (pdf) or a mixture of discrete and continuous (e.g. thresholded or censored data)
- Likelihood function $L(\theta)=\prod_{i=1}^{n} f_{i}\left(Y_{i} ; \theta\right)$. (assumes independent - otherwise, joint density fo the observations)
- Maximum likelihood estimator (MLE) chooses $\hat{\theta}$ to maximize $L(\theta)$ or equivalently to minimize $\ell(\theta)=-\sum_{i=1}^{n} \log f_{i}\left(Y_{i} ; \theta\right)$.


## Variances, Covariances, Standard Errors

- Notation: $\frac{\partial^{2} \ell}{\partial \theta \partial \theta^{T}}$ matrix of second-order derivatives $((i, j)$ entry is $\left.\frac{\partial^{2} \ell}{\partial \theta_{i} \partial \theta_{j}}\right)$.
- Let $H(\theta)$ be $\frac{\partial^{2} \ell}{\partial \theta \partial \theta^{T}}$ (Hessian matrix) and let $I(\theta)$ be the expected value of $H(\theta)$
- Usually, $H(\theta)$ is evaluated at the MLE $\hat{\theta}$ and $I(\theta)$ is evaluated at the true value, say $\theta^{*}$. Then $I$ is the Fisher Information Matrix and $H$ is the Observed Information Matrix
- Either of the inverses, $I^{-1}$ or $H^{-1}$ is a good approximation to the variance-covariance matrix of $\widehat{\theta}$ but $H^{-1}$ is easier to compute
- The square roots of the diagonal entries of $H^{-1}$ are the (estimated) standard errors of the parameter estimates
- Aside: No connection with the hat matrix


## Model Selection: Nested Case

- Suppose we want to compare two models $\omega$ and $\Omega$, where $\omega$ is a subset of $\Omega, p_{\omega}<p_{\Omega}$ parameters
- Let $\hat{\theta}_{\omega}, \hat{\theta}_{\Omega}$ be the parameter estimates under both models
- $D=2\left\{\ell\left(\theta_{\omega}\right)-\ell\left(\theta_{\Omega}\right)\right\}>0$ is called the deviance
- If $H_{0}: \omega$ is true then the distribution of $D$ is approximately $\chi_{p_{\Omega}-p_{\omega}}^{2}$ - analogous to the F-test for ANOVA.
- This is the likelihood ratio test (LRT). The text (Appendix A2, page 378) discusses two other tests, the Wald test and the score test, but the LRT is the one most used.


## Model Selection: Comparing Many Models

- In practice, not all models are nested, and even if they were, doing many hypothesis tests is not usually a good idea (multiple testing or "data snooping" problem)
- Alternatives use automated selection criteria. Example are:
- AIC: minimize $2 \ell(\hat{\theta})+2 p$
- BIC: minimize $2 \ell(\hat{\theta})+p \log n$
- DIC: minimize $D(\bar{\theta})+2 p_{D}$ where $D$ is deviance, $p_{D}=$ $D(\theta)-D(\bar{\theta})$ and $\overline{\text { ? denotes the mean }}$
- Note: Faraway uses $\ell$ to denote the log likelihood, whereas I have used it for the negative log likelihood.


## Example 1: Linear Regression with known $\sigma^{2}$

- $f\left(y_{i} ; \beta\right) \propto \exp \left\{-\frac{1}{2 \sigma^{2}}\left(y_{i}-\sum_{j} x_{i j} \beta_{j}\right)^{2}\right\}$
- Ignoring constants, $\ell(\beta)=\frac{1}{2 \sigma^{2}} \sum_{i}\left(y_{i}-\sum_{j} x_{i j} \beta_{j}\right)^{2}$
- $\frac{\partial \ell}{\partial \beta_{k}}=\frac{1}{\sigma^{2}} \sum_{i} x_{i k}\left(y_{i}-\sum_{j} x_{i j} \beta_{j}\right)$
- $\frac{\partial^{2} \ell}{\partial \beta_{k} \partial \beta_{m}}=\frac{1}{\sigma^{2}} \sum_{i} x_{i k} x_{i m}$
- Setting $\frac{\partial \ell}{\partial \beta_{k}}=0$ for all $k$ gives the standard normal equations
- $H(\beta)$ or $I(\beta)$ are both $\frac{1}{\sigma^{2}} X^{T} X$ so they lead to the standard formula $\sigma^{2}\left(X^{T} X\right)^{-1}$ for the variance-covariance matrix of $\widehat{\beta}$.


## Example 2:

## Logistic Regression With One Covariate

- $f_{i}\left(y_{i} ; \theta\right)=\frac{\exp \left\{y_{i}\left(\beta_{0}+\beta_{1} x_{i}\right)\right\}}{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}, \theta=\left(\beta_{0}, \beta_{1}\right)$
- $\ell=\sum_{i} \log \left\{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)\right\}-\sum_{i} y_{i}\left(\beta_{0}+\beta_{1} x_{i}\right)$
- $\frac{\partial \ell}{\partial \beta_{0}}=\sum_{i} \frac{\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}-\sum_{i} y_{i}$
- $\frac{\partial \ell}{\partial \beta_{1}}=\sum_{i} \frac{x_{i} \exp \left(\beta_{0}+\beta_{1} x_{i}\right)}{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}-\sum_{i} x_{i} y_{i}$
- Set $\frac{\partial \ell}{\partial \beta_{0}}=\frac{\partial \ell}{\partial \beta_{1}}=0$, solve for $\beta_{0}, \beta_{1}$
- Intuition: $\sum_{i}\left(y_{i}-p_{i}\right)=0, \sum_{i} x_{i}\left(y_{i}-p_{i}\right)=0$
- Even so, the equations are nonlinear - solve numerically for $\widehat{\beta}_{0}, \widehat{\beta}_{1}$
- Rewrite $\frac{\partial \ell}{\partial \beta_{0}}=\sum_{i}\left(1-\frac{1}{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}\right)-\sum_{i} y_{i}$,

$$
\frac{\partial \ell}{\partial \beta_{1}}=\sum_{i} x_{i}\left(1-\frac{1}{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)}\right)-\sum_{i} x_{i} y_{i}
$$

- $\frac{\partial^{2} \ell}{\partial \beta_{0}^{2}}=\sum_{i}\left\{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)\right\}^{-2} \cdot \exp \left(\beta_{0}+\beta_{1} x_{i}\right)>0$
- Also write as $\sum_{i} p_{i}\left(1-p_{i}\right)$
- $\frac{\partial^{2} \ell}{\partial \beta_{1}^{2}}=\sum_{i} x_{i}^{2}\left\{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)\right\}^{-2} \cdot x_{i}^{2} \exp \left(\beta_{0}+\beta_{1} x_{i}\right)>0$
- $\frac{\partial^{2} \ell}{\partial \beta_{0} \partial \beta_{1}}=\sum_{i} x_{i}\left\{1+\exp \left(\beta_{0}+\beta_{1} x_{i}\right)\right\}^{-2} \cdot x_{i} \exp \left(\beta_{0}+\beta_{1} x_{i}\right)$
- $H=\left[\begin{array}{cc}\sum_{i} \widehat{p}_{i}\left(1-\widehat{p}_{i}\right) & \sum_{i} x_{i} \hat{p}_{i}\left(1-\widehat{p}_{i}\right) \\ \sum_{i} x_{i} \widehat{p}_{i}\left(1-\widehat{p}_{i}\right) & \sum_{i} x_{i}^{2} \widehat{p}_{i}\left(1-\widehat{p}_{i}\right)\end{array}\right]$
- The determinant of $H$ is $>0$ unless all the $x_{i}$ are the same - this proves that ( $\widehat{\beta}_{0}, \widehat{\beta}_{1}$ ) is a local minimum of $\ell$ and $H^{-1}$ is a good approximation to the variance-covariance matrix of ( $\widehat{\beta}_{0}, \widehat{\beta}_{1}$ )


## Interpretation as Ratio of Odds

- Example: For the smoking-CHD example in the text, $\widehat{\beta}_{2}=$ 0.02313 . How should this be interpreted?
- One answer: for a person who smokes 20 cigarettes a day, $\log \frac{p}{1-p}$ is $20 \times 0.02313=0.4626$ larger than for a person who smokes none ( $p$ : probability of CHD)
- Alternatively: for a person who smokes 20 cigarettes a day, $\frac{p}{1-p}$ is multiplied by $e^{0.4626}=1.59$
- In common probability terminology, $\frac{p}{1-p}$ is the odds.
- Example: One bookmaker gives odds of 37:20 that the Patriots will win the Superbowl.
- Equivalent to: probability of winning is $\frac{37}{37+20}=0.65$.
- For a $20-a-d a y ~ s m o k e r, ~ o d d s ~ o f ~ C H D ~ a r e ~ i n c r e a s e d ~ b y ~ 59 \% . ~$
- Almost the same as: the risk of CHD is increased by $59 \%$.


## Deviance Residuals

- Define the deviance as

$$
\begin{aligned}
D & =2 \ell(\widehat{\theta}) \\
& =2 \sum_{i}\left[\log \left\{1+\exp \left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right)\right\}-y_{i}\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right)\right] \\
& =\sum_{i} r_{i}^{2}
\end{aligned}
$$

where

$$
r_{i}^{2}=2\left[\log \left\{1+\exp \left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right)\right\}-y_{i}\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right)\right]
$$

Ensure correct sign by defining

$$
r_{i}=\operatorname{sign}\left(y_{i}-\hat{p}_{i}\right) \sqrt{r_{i}^{2}}
$$

We call $r_{i}$ the $i$ 'th deviance residual (text, page 36 ).
In R: residuals(lmod)

## Side Comment

- We defined

$$
r_{i}^{2}=2\left[\log \left\{1+\exp \left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right)\right\}-y_{i}\left(\widehat{\beta}_{0}+\widehat{\beta}_{1} x_{i}\right)\right]
$$

Do we know this is $>0$ ?

- Claim: $\log \left(1+e^{z}\right)-y z>0$ when $-\infty<z<\infty, y=0$ or 1
- $y=0: \log \left(1+e^{z}\right)>\log (1)>0$
- $y=1: \log \left(1+e^{z}\right)-z>\log \left(e^{z}\right)-z=0$
- So OK either way.


## Profile Likelihood

- Sometimes we're primarily interested in one parameter - all the rest are "nuisance parameters"
- Say $\theta_{1}$ is interest parameter, $\theta_{2}, \ldots, \theta_{p}$ are nuisance
- Define

$$
\ell_{P}\left(\theta_{1}^{*}\right)=\min \left\{\ell\left(\theta_{1}, \ldots, \theta_{p}\right): \theta_{1}=\theta_{1}^{*}\right\}
$$

- This is called the profile (log) likelihood of $\theta_{1}$
- Can test a specific value for $\theta_{1}^{*}$ by using LRT with $\chi_{1}^{2}$ distribution


## Example: Box-Cox Transformation

- Produced in R via library(MASS) followed by boxcox(lmod) where Imod is fitted model
- Plots profile likelihood of the Box-Cox transformation parameter $\lambda$
- The dotted line is 3.84 below the maximum.
- 3.84 is the $95^{\text {th }}$ percentile of the chi-square distribution with 1 DF
- Interpretation: every $\lambda$ whose profile likelihood is above the dotted line is accepted by the hypothesis test at significance level 0.05. In other words, this defines the 95\% confidence interval.
- Same idea is used for the "confint" command for a glm


