#### Reference: Agresti, Sections 5.2-5.5

• The logistic regression model is defined as

$$\operatorname{logit}(\pi_i) = \operatorname{log}\left(\frac{\pi_i}{1 - \pi_i}\right) = \boldsymbol{x}_i' \boldsymbol{\beta},$$

•  $\beta_j$  represents the **change in log-odds** resulting from a one-unit increase in  $x_{ij}$ , holding all other covariates constant.

• The coefficients  $\beta_j$ 's correspond to log-odds ratios.

• The logit transformation is one-to-one

$$\pi_i = \operatorname{logit}^{-1}(\eta_i) = \frac{e^{\eta_i}}{1 + e^{\eta_i}} = \frac{e^{\boldsymbol{x}_i'}\boldsymbol{\beta}}{1 + e^{\boldsymbol{x}_i'}\boldsymbol{\beta}}.$$

• This is an S-shaped function. As  $\boldsymbol{x}_i$  increases,  $\pi_i$  increases when  $\beta > 0$ , and  $\pi_i$  decreases when  $\beta < 0$ .

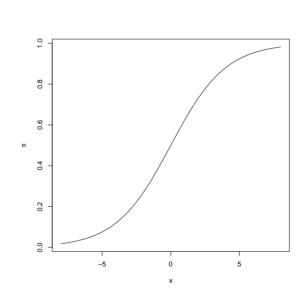


Figure 1: Logistic regression function,  $\beta > 0$ 

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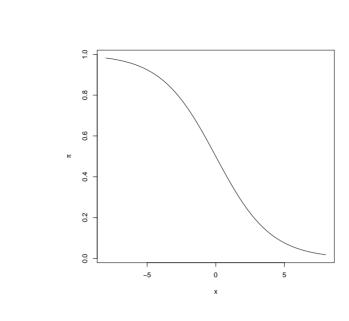


Figure 2: Logistic regression function,  $\beta<0$ 

### Maximum likelihood estimation

- Since the logit is the canonical link for binomial data, Newton-Raphson and Fisher scoring are the same.
- We iterate until convergence

$$oldsymbol{eta}^{(t+1)} = oldsymbol{eta}^{(t)} + \left( oldsymbol{X}' oldsymbol{W} oldsymbol{X} 
ight)^{-1} oldsymbol{X}' \left( oldsymbol{y} - oldsymbol{\mu}^{(t)} 
ight),$$

where

$$\mu_i^{(t)} = n_i \pi_i^{(t)}, \quad \mathbf{W}^{(t)} = \text{Diag}(n_i \pi_i^{(t)} (1 - \pi_i^{(t)})),$$

$$\pi_i^{(t)} = \frac{e^{\mathbf{x}_i'} \boldsymbol{\beta}^{(t)}}{1 + e^{\mathbf{x}_i'} \boldsymbol{\beta}^{(t)}}.$$

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• We could also use the iterative re-weighted least squares approach

$$oldsymbol{eta}^{(t)} = \left( oldsymbol{X}' oldsymbol{W}^{(t)} oldsymbol{X} 
ight)^{-1} oldsymbol{X}' oldsymbol{W}^{(t)} oldsymbol{z}^{(t)},$$

where the working dependent variable  $z^{(t)}$  has elements

$$z_i^{(t)} = \eta_i^{(t)} + \frac{y_i - \mu_i^{(t)}}{\mu_i^{(t)} (n_i - \mu_i^{(t)})} n_i.$$

• With large samples

$$\hat{\boldsymbol{\beta}} \stackrel{d}{\longrightarrow} N(\boldsymbol{\beta}, (\boldsymbol{X}'\widehat{\boldsymbol{W}}\boldsymbol{X})^{-1}).$$

#### Wald test

• We can test  $H_0: \beta_j = 0$  using the Wald test

$$z = \frac{\hat{\beta}_j}{\sqrt{\widehat{var}(\hat{\beta}_j)}} \xrightarrow{d} N(0,1),$$

where  $\widehat{var}(\hat{\beta}_j)$  is the (j, j)-th element of  $\widehat{Var}(\hat{\beta})$ .

• The Wald test can be used to derive a confidence interval for  $\beta_j$ 

$$\hat{\beta}_j \pm z_{1-\alpha/2} \sqrt{\widehat{var}(\hat{\beta}_j)},$$

• The Wald test can be applied to test hypotheses concerning several coefficients

$$W = (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)' \widehat{Var}^{-1} (\hat{\boldsymbol{\beta}}) (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) \stackrel{d}{\longrightarrow} \chi^2_{\dim(\beta)}.$$

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#### Likelihood ratio test

• Consider partitioning the model matrix and the vector of coefficients into two components

$$m{X} = (m{X}_1, m{X}_2) \quad ext{and} \quad m{eta} = \left(egin{array}{c} m{eta}_1 \ m{eta}_2 \end{array}
ight)$$

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with  $p_1$  and  $p_2$  elements, respectively.

• Consider testing the hypothesis

$$H_0: \boldsymbol{\beta}_2 = 0.$$

• Let  $D(X_1)$  and  $D(X_1 + X_2)$  denote respectively the deviances of a model with  $X_1$  and a model with all variables in X

$$D(\boldsymbol{X}_1) - D(\boldsymbol{X}_1 + \boldsymbol{X}_2) \stackrel{d}{\longrightarrow} \chi_{p_2}^2$$

#### Inference on functions of $\beta$

• By the delta method, we have

$$g(\hat{\boldsymbol{\beta}}) \sim N\left(g(\boldsymbol{\beta}), \left(\frac{\partial g(\hat{\boldsymbol{\theta}})}{\partial \boldsymbol{\beta}}\right)^T \ \widehat{Var}(\hat{\boldsymbol{\beta}}) \ \left(\frac{\partial g(\hat{\boldsymbol{\theta}})}{\partial \boldsymbol{\beta}}\right)\right).$$

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• One important non-linear function is  $\pi$ 

$$\pi_i = \frac{e^{\boldsymbol{x}_i'\boldsymbol{\beta}}}{1 + e^{\boldsymbol{x}_i'\boldsymbol{\beta}}}.$$

#### Fitted values

• Verify that an estimated variance for  $\hat{\pi}_i$  is

$$\widehat{Var}(\hat{\pi}_i) = \hat{\pi}_i^2 (1 - \hat{\pi}_i)^2 \boldsymbol{x}_i' \left( \boldsymbol{X}' \widehat{\boldsymbol{W}} \boldsymbol{X} \right)^{-1} \boldsymbol{x}_i.$$

• Define  $U = \text{Diag}(\pi_i(1 - \pi_i))$ , then

$$\widehat{Var}(\widehat{\boldsymbol{\pi}}) = \boldsymbol{U}\boldsymbol{X} \left( \boldsymbol{X}' \widehat{\boldsymbol{W}} \boldsymbol{X} \right)^{-1} \boldsymbol{X}' \boldsymbol{U}.$$

• Since this estimate borrows information across the entire dataset  $y_1, \ldots, y_N$ , it should be smaller than the estimated variance of  $p_i = y_i/n_i$ ,  $\widehat{Var}(p_i) = p_i(1-p_i)/n_i$ , provided the model is true.

#### Testing goodness-of-fit

• In logistic regression, the fitted values are

$$\hat{\mu}_i = n_i \hat{\pi}_i = n_i \frac{\exp(\boldsymbol{x}_i' \hat{\boldsymbol{\beta}})}{1 + \exp(\boldsymbol{x}_i' \hat{\boldsymbol{\beta}})}, \quad i = 1, \dots, N.$$

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- The deviance  $G^2$  and the Pearson  $\mathcal{X}^2$  compare the fitted values  $\hat{\mu}_i$ 's to the  $y_i$ 's.
- That is, these statistics test the fit of the logit model (a p-parameter model) against the saturated model that allows  $\pi_i$  to lie anywhere in (0,1) (an N-parameter model).

#### Deviance test statistic

• The deviance test statistic is

$$G^{2} = 2\sum_{i=1}^{N} \left\{ y_{i} \log \left( \frac{y_{i}}{\hat{\mu}_{i}} \right) + (n_{i} - y_{i}) \log \left( \frac{n_{i} - y_{i}}{n_{i} \hat{\mu}_{i}} \right) \right\} \xrightarrow{d} \chi_{N-p}^{2}.$$

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- As the group sizes  $n_i \to \infty$ ,  $\forall i$ , the deviance statistic converges to  $\chi^2_{N-p}$ , where N is the number of groups and p is the number of parameters in the model (including the intercept).
- With individual data, the distribution of the deviance does not converge to a chi-squared and it can not be used as a goodness-of-fit test.

#### Pearson goodness-of-fit statistic

• The **Pearson residuals** are defined as

$$e_i = \frac{y_i - \hat{\mu}_i}{\sqrt{\widehat{Var}(\hat{\mu}_i)}} = \frac{y_i - n_i \hat{\pi}_i}{\sqrt{n_i \hat{\pi}_i (1 - \hat{\pi}_i)}}$$

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• The Pearson goodness-of-fit statistic is

$$\mathcal{X}^2 = \sum_{i}^{N} e_i^2 \xrightarrow{d} \chi_{N-p}^2.$$

- With grouped data and large samples, the Pearson  $\mathcal{X}^2$  statistic has a  $\chi^2_{N-p}$  distribution and is equivalent to the deviance.
- It cannot be used as a goodness of fit test with individual data.

```
Let's revisit the Beetles data.
            Beetles$alive = Beetles$n - Beetles$dead
            attach(Beetles)
            fit.logit = glm(cbind(dead, alive) ~ logdose, family=binomial(link=logit))
            summary(fit.logit)
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            Coefficients:
                       Estimate Std. Error z value Pr(>|z|)
            (Intercept) -60.740 5.182 -11.72 <2e-16 ***
                       34.286 2.913 11.77 <2e-16 ***
            logdose
            ___
            Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
                Null deviance: 284.202 on 7 degrees of freedom
            Residual deviance: 11.116 on 6 degrees of freedom
                            Goodness-of-fit statistics
```

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sum(resid(fit.logit, type="pearson")^2) [1] 9.906715 
# p-values 
1-pchisq(11.116, 6); 1-pchisq(9.906715, 6) [1] 0.0848568 
[1] 0.1286358 
The deviance  $G^2 = 11.12$  and Pearson  $\chi^2 = 9.91$  have df = 8 - 2 = 6 and show slight evidence of lack-of-fit (p-values  $\approx 0.1$ ).

Residual deviance: 11.116 on 6 degrees of freedom

# Pearson chi-squared goodness-of-fit, df=6

# Deviance test statistic

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A 0.1 unit increase in  $\log_{10}$ -concentration

- increases the log-odds of death by 3.4286
- is associated with a log-odds ratio of 3.4286
- multiplies the odds of death by  $\exp(3.4286) = 30.83$ .

# Obtaining fitted values and residuals

```
pihat.logit = fit.logit$fitted.values
                                               # fitted values
pearson.res = resid(fit.logit, type="pearson")
                                                       # Pearson residuals
```

# Slide 16

logdose pihat.logit pearson.res 1 1.691 0.1016949 0.05937747 1.3753932 2 1.724 0.2166667 0.16366723 1.1096257 3 1.755 0.2903226 0.36162283 -1.1684774 4 1.784 0.5000000 0.60490961 -1.6058900 5 1.811 0.8253968 0.79440490 0.6086835 1.837 0.8983051 0.90405532 -0.1499696

> cbind(logdose, dead/n, pihat.logit, pearson.res)

6

7 1.861 0.9838710 0.95546748 1.0842287

1.884 1.0000000 0.97925643 8 1.1273769

#### Hosmer-Lemeshow goodness-of-fit statistic

- Hosmer and Lemeshow (1989) have proposed a procedure that can be used with individual data even if there are no common covariate patterns.
- Hosmer-Lemeshow recommend forming ten groups with predicted probabilities  $(0-0.1], (0.1-0.2], \ldots, (0.9,1)$ .
- Other ways of pooling the data can be considered.
- One can then compute expected counts for each group and compare them with the observed values

$$\chi_{HL}^2 = \sum_{i=1}^{G} \frac{\left[ \left( \sum_{j} y_{ij} - \sum_{j} \hat{\pi}_{ij} \right)^2}{\left( \sum_{j} \hat{\pi}_{ij} \right) \left[ 1 - \left( \sum_{j} \hat{\pi}_{ij} \right) / n_i \right]}$$

 $y_{ij} = \text{binary outcome for observation } j \text{ in group } i$  $\hat{\pi}_{ij} = \text{fitted probability for ungrouped data.}$ 

#### Hosmer-Lemeshow goodness-of-fit statistic

- The statistic does not have a chi-squared distribution, but simulation studies have shown that in large samples it is similar to a chi-squared distribution with df = G 2.
- A large value of the Hosmer-Lemeshow statistic indicates some lack of fit but does not provide insight about its nature.

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# Example: Low birth weight (saved as BirthWeight.txt)

ID	Identification code
LOW	Low birth weight (0=weight>2500g, 1=weight<2500g)
AGE	Age of mother in years
LWT	Weight in pounds at last menstrual period
RACE	Race (1=White, 2=Black, 3=Other)
SMOKE	Smoking status during pregnancy (1=Yes, 0=No)
PTL	History of premature labor (0=None, 1=One, 2=Two, etc.
HT	History of hypertension (1=Yes, 0=No)
UI	Presence of uterine irritability (1=Yes, 0=No)
FTV	Number of physician visits during the first trimester
BWT	Birth weight in grams

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- We want to model the risk of low birthweight (low=1) in terms of maternal pre-pregnancy weight (lwt), race, smoking status, history of premature labor (ptl) and history of hypertension (ht).
- Very few observations share the same lwt value, so there will be one observation in most of the cells created by covariate patterns.

```
attach(BrithWeight)
bwt.logit = glm(low ~ lwt+smoke+as.factor(race)+ptl+ht, family="binomial")

library(ResourceSelection)
res = hoslem.test(bwt.logit$y, fitted(bwt.logit))

> res
Hosmer and Lemeshow goodness of fit (GOF) test
data: bwt.logit$y, fitted(bwt.logit)
```

# Slide 22

```
      y0
      y1
      yhat0
      yhat1

      [0.038,0.104]
      18
      1
      17.611209
      1.388791

      (0.104,0.14]
      16
      3
      16.739105
      2.260895

      (0.14,0.199]
      14
      5
      15.816089
      3.183911

      (0.199,0.261]
      16
      3
      14.473849
      4.526151

      (0.261,0.284]
      18
      2
      14.474378
      5.525622

      (0.284,0.322)
      9
      8
      11.795959
      5.204041

      (0.322,0.361)
      12
      7
      12.549143
      6.450857

      (0.361,0.442)
      12
      7
      11.610390
      7.389610

      (0.442,0.603)
      10
      9
      9.202104
      9.797896

      (0.603,0.837)
      5
      14
      5.727773
      13.272227
```

X-squared = 7.9557, df = 8, p-value = 0.4378

> cbind(res\$observed, res\$expected)

Thus, the model appears to be adequate for these data, so we can go ahead and look at the parameter estimates:

> summary(bwt.logit)

#### Coefficients:

#### Estimate Std. Error z value Pr(>|z|)(Intercept) 0.117888 0.944152 0.125 0.9006 lwt -0.016580 0.006857 -2.418 0.0156 \* smoke 0.946179 0.394947 2.396 0.0166 \* as.factor(race)2 1.290381 0.522377 2.470 0.0135 \* as.factor(race)3 0.910325 0.428269 2.126 0.0335 \* ptl 0.602481 0.335233 1.797 0.0723 . 1.745050 0.694902 2.511 0.0120 \* ht

Null deviance: 234.67 on 188 degrees of freedom Residual deviance: 204.90 on 182 degrees of freedom

#### Is grouping a good idea?

- If the model is true, adding the  $y_i$ 's causes no loss of information.
- If the model is not true (e.g. important covariates omitted), then two models with same  $x_i$ 's may have different  $\pi_i$ 's.
- Grouping may sacrifice our ability to detect departures from the model.

### Slide 23