### Binomial Regression I

Binomial Regression I

### Learning goals

Understand binomial regression

- know when you should use binormal regression.
- be able to write binomial regression model and its likelihood.
- be able to obtain estimators of parameters or function of parameters using R script.
- be able to quantify uncertainty of the estimators (e.g., computing CI).
- be able to test hypothesis.
- be able to do model selection.

Understand asymptotic properties of MLEs (maximum likelihood estimators)

• use asymptotic normality of MLEs to quantify uncertainty of the estimators (e.g., Wald CI).

Undertand Wald test and likelihood ratio test (LRT)

• use them to test hypothesis in binomial regression

Understand (scaled) deviance

• use it to test model adequacy or perform LRT and model comparison.

# Challenger example

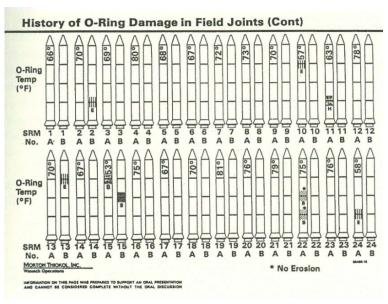
### Challenger disaster

On the 28th of January 1986 the Space Shuttle Challenger broke apart after an O-ring seal failed at liftoff, leading to the deaths of its seven crew members.

Despite concerns about the O-rings failing due to the cold—the forecast temperature was  $29 \pm 3$  °F—no one was able to provide an analysis that convinced NASA (who were under pressure to launch following several previous delays) not to go ahead.

The way the data was presented didn't help matters.

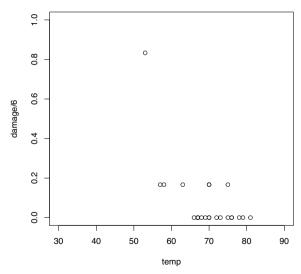
### Challenger disaster: data



### Challenger disaster: data

Summarise data using number of damaged O-rings (out of 6) per launch. Data is in dataframe orings. Response damage is number of damaged O-rings (out of 6). Predictor temp is temperature (°F) > library(faraway) > data(orings) > str(orings) data.frame: 23 obs. of 2 variables: \$ temp : num 53 57 58 63 66 67 67 67 68 69 ... \$ damage: num 5 1 1 1 0 0 0 0 0 0 ... > plot(damage/6 ~ temp, data = orings, xlim = c(30, 90), ylim = c(0, 1)

### Challenger disaster: visualize data



### Challenger disaster: model

Make the assumption that  $Y_i$ , the number of damaged O-rings on the i-th launch, has distribution

$$Y_i \sim \mathsf{bin}(6, p_i)$$

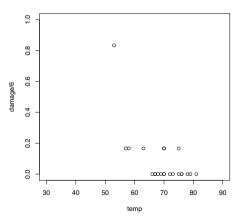
where  $p_i$  depends on the temperature  $t_i$ . We also assume that the  $Y_i$  are independent.

How to relate  $p_i$  with  $t_i$ .

• Question: just use a linear relationship?  $p_i = \beta_0 + \beta_1 t_i$ ?

No. We need parameter bounds so  $0 \le p_i \le 1$ . We need alternate function to relate  $p_i$  with  $t_i$ .

Alternative function to relate  $p_i$  with  $t_i$  for a single launch, best estimate of  $p_i$  is just  $y_i/6$ . From plot of  $y_i/6$  against  $t_i$  it is reasonable to assume that  $p_i = p(t_i)$  where p is a smooth function of the temperature, decreasing from 1 down to 0 as the temperature increases.



We choose logistic function: suppose that for some  $\beta_0$  and  $\beta_1$ 

$$ho(t) = rac{1}{1 + e^{-(eta_0 + eta_1 t)}} = rac{e^{eta_0 + eta_1 t}}{1 + e^{eta_0 + eta_1 t}}$$

• Restricts  $0 \le p(t) \le 1$ 

Monotonic increasing/decreasing function

Can be linearized through the *logit* transformation

$$\log \frac{\rho(t)}{1 - \rho(t)} = \beta_0 + \beta_1 t$$

We choose logistic function: suppose that for some  $\beta_0$  and  $\beta_1$ 

$$p(t) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 t)}} = \frac{e^{\beta_0 + \beta_1 t}}{1 + e^{\beta_0 + \beta_1 t}}$$

$$p(t) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 t)}} \Rightarrow 0 + p(t) = \frac{e^{\beta_0 + \beta_1 t}}{1 + e^{\beta_0 + \beta_1 t}}$$

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$$p(t) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 t)}} \Rightarrow 0 + p(t) = \frac{e^{\beta_0 + \beta_1 t}}{1 + e^{\beta_0 t}}$$

- curve.
- $p'(-\beta_0/\beta_1) = \beta_1/4$ , so  $\beta_1$  controls the steepness of the curve.

Example: see R script and result in the section "logistic function with different values for beta0 and beta1" of Challenger.pdf.



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### Challenger disaster: model

Make the assumption that  $Y_i$ , the number of damaged O-rings on the *i*-th launch, has distribution

$$Y_i \sim \text{bin}(6, p_i)$$

where

$$p_i = rac{e^{eta_0 + eta_1 t_i}}{1 + e^{eta_0 + eta_1 t_i}}.$$
 parameter: for  $k$  for

We also assume that the  $Y_i$  are independent.

### Challenger disaster: model fitting

Make the assumption that  $Y_i$ , the number of damaged O-rings on the i-th launch, has distribution

$$Y_i \sim \text{bin}(6, p_i)$$

where

$$p_i = \frac{e^{\beta_0 + \beta_1 t_i}}{1 + e^{\beta_0 + \beta_1 t_i}}.$$

We also assume that the  $Y_i$  are independent.

Maximum likelihood estimators (MLE)  $\hat{\beta}_0$ ,  $\hat{\beta}_1$ : values for  $\beta_0$ ,  $\beta_1$  which maximize the log-likelihood.

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## Challenger disaster: model fitting

The log-likelihood is

$$I(\beta_{0},\beta_{1}) = \log \mathcal{L}(\beta_{0},\beta_{1})$$

$$= \log \mathbb{P}(Y = y \mid \beta_{0},\beta_{1}) = \log \prod_{i} \mathbb{P}(Y_{i} = y_{i} \mid \beta_{0},\beta_{1})$$

$$= \sum_{i} \log \left( \binom{6}{y_{i}} p_{i}^{y_{i}} (1 - p_{i})^{6 - y_{i}} \right)$$

$$= c + \sum_{i} \left( y_{i} \log p_{i} + (6 - y_{i}) \log(1 - p_{i}) \right)$$

$$= c + \sum_{i} \left( y_{i} \log \frac{p_{i}}{1 - p_{i}} + 6 \log(1 - p_{i}) \right)$$

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$$\frac{1}{1-\frac{1}{1+e^{-n}}}$$

$$=\frac{1}{1+e^{-n}}$$

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### Challenger disaster: model fitting

There is no closed form solution for MLE  $\hat{\beta}_0$ ,  $\hat{\beta}_1$  in this model. Numerical search procedures are required to find MLE.

- the glm function uses the iterative weighted least squares (IWLS) algorithm I will cover this later.
- For now, let's use the optim function.

### Example:



- See R script and result in "maximum likelihood fitting" of Challenger.pdf
- $\hat{\beta}_0 = 11.667 \text{ and } \hat{\beta}_1 = -0.216$

### Challenger disaster: questions

- Forecast probability of an O-ring being damaged when the launch temperature is 29 °F.
- How good is our forecast? Can we provide a confidence interval?
- Is temperature useful to predict the O-ring failing?

linear model 
$$y_i = \beta_0 + \beta_1 \times i + 2i$$
  $z_i \times N(0, \sigma^2)$   
 $\beta_i$   $\beta_1 \times N(\beta_1, se(\beta_1))$   $95\% CI for  $\beta_1 = \beta_1 + 2\beta_1 \cdot se(\beta_1)$$ 

# Binomial regression

### Binomial regression model

## Vi independen

We suppose that we observe  $Y_i \sim \text{bin}(m_i, p_i)$ , i = 1, ..., n, independent.

The  $m_i$  are known and we suppose that for some **link function**  $g_i$ 

$$g(p_i) = \eta_i = \mathbf{x}_i^T \boldsymbol{\beta} = \beta_0 + \beta_1 \mathbf{x}_{i1} + \dots + \beta_q \mathbf{x}_{iq}$$

where  $x_i$  are known predictors and  $\beta$  are unknown parameters.

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### Binomial regression model: link function

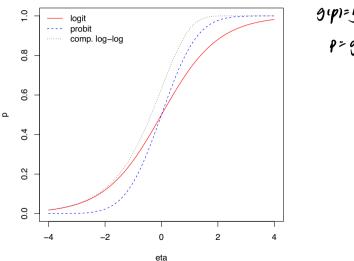
where  $\Phi$  is the cumulative distribution function (cdf) of the standard normal distribution.

Binomial Regression I

### Binomial regression model: link function

### Binomial regression model: link function

#### binomial link functions



### Binomial regression model: likelihood

Given observations  $y_i$  of  $Y_i \sim \text{bin}(m_i, p_i = g^{-1}(\eta_i))$ , where  $\eta_i = x_i^T \beta$ , the log-likelihood is

$$I(\beta) = \sum_{i=1}^{n} \log \mathbb{P}(Y_i = y_i)$$

$$= \sum_{i=1}^{n} \log \left( \binom{m_i}{y_i} p_i^{y_i} (1 - p_i)^{m_i - y_i} \right)$$

$$= c + \sum_{i=1}^{n} y_i \log(g^{-1}(\eta_i)) + (m_i - y_i) \log(1 - g^{-1}(\eta_i))$$

There is no closed form solution for MLE of  $\beta$ . Numerical search procedures are required to find MLE.

Binomial Regression I

### Reminder: questions from Challenger disaster

- Forecast probability of an O-ring being damaged when the launch temperature is 29 °F.
- How good is our forecast? Can we provide a confidence interval?
- Is temperature useful to predict the O-ring failing?

# Forecast probability of an O-ring being damaged when the launch temperature is $29 \, {}^{\circ}F$ .

$$\hat{p} = g^{-1}(\hat{\eta})$$
 when  $t = 29$ .

$$\hat{
ho} = rac{\exp(\hat{\eta})}{1+\exp(\hat{\eta})}$$
, where  $\hat{\eta} = \hat{eta}_0 + \hat{eta}_1$ 29

 $\hat{p}=0.995$  : see R script and result in "prediction for temp of 29" of Challenger.pdf

### Reminder: questions from Challenger disaster

- Forecast probability of an O-ring being damaged when the launch temperature is 29 °F.
- How good is our forecast? Can we provide a confidence interval?
- Is temperature useful to predict the O-ring failing?

We need to know properties of MLE!!

# Asymptotic properties MLE

### Reminder: Maximum likelihood estimate (MLE)

Suppose that  $Y_i$ , i = 1, ..., n, are independent, with densities/mass-functions  $f_i(\cdot; \theta)$ .

Given observations  $y_i$  of the  $Y_i$ , the log-likelihood is

$$I(\theta) = I(\theta; y) = \sum_{i} \log f_i(y_i; \theta),$$

MLE  $\hat{\theta}$  is that value of  $\theta$  which maximises  $l(\theta)$ .

Note that allowing  $f_i$  to depend on i means that we can include the case where the distribution of  $Y_i$  depends on some covariate  $x_i$ . That is, we can have  $f_i(\cdot; \theta) = f(\cdot; x_i, \theta)$  for some common f.

Binomial Regression I

### Asymptotic properties of MLE

n→ 10

Under certain regularity conditions (to be introduced later), the MLE is

- asymptotically consistent,
- asymptotically normal,
- asymptotically efficient.

### MLE: asymptotic consistency

Let 
$$\underline{\theta^*}$$
 denote a true value for  $\underline{\theta}$ . As  $n \to \infty$ ,  $\hat{\theta} \stackrel{\mathrm{p}}{\longrightarrow} \underline{\theta^*}$ . That is for any  $\epsilon > 0$  
$$\underline{\mathbb{P}}(|\hat{\theta} - \theta^*| > \epsilon) \to 0 \text{ as } n \to \infty.$$

Let  $\theta^*$  denote a true value for  $\theta$ .

$$\hat{m{ heta}} pprox^d N(m{ heta}^*, \mathcal{I}(m{ heta}^*)^{-1})$$

The observed information is

2 2nd partial destinative of log whether A

$$\mathcal{J}(\boldsymbol{\theta}) = -\frac{\partial^2 I(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T} = -\mathsf{H}_{I(\boldsymbol{\theta})},$$

where the hessian matrix,  $H_{l(\theta)}$ , is a square matrix of second-order partial derivatives of the log likelihood.

For binomial regression with one predictor (e.g.,  $\theta = \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$ ):

$$\mathcal{J}(oldsymbol{ heta}) = \mathcal{J}(oldsymbol{eta}) = egin{pmatrix} -rac{\partial^2 l(oldsymbol{eta})}{\partial eta_0^2} & -rac{\partial^2 l(oldsymbol{eta})}{\partial eta_1 \partial eta_0} \ -rac{\partial^2 l(oldsymbol{eta})}{\partial eta_0 \partial eta_1} & -rac{\partial^2 l(oldsymbol{eta})}{\partial eta_1^2} \end{pmatrix}$$

Clearly  $\mathcal{J}(\theta) = \mathcal{J}(\theta; y)$  depends on y through  $I(\theta) = I(\theta; y)$ .

The Fisher information is

observed information

$$\mathcal{I}(\boldsymbol{\theta}) = \mathbb{E}[\underbrace{\mathcal{I}(\boldsymbol{\theta};\mathsf{Y})}_{\bullet}.$$

 $\mathcal{I}( heta)$  does not depend on y. ightharpoonup since we did expertation

Binomial Regression I

### Exercise: binomial regression with a logit link

We suppose that we observe  $Y_i \sim \text{bin}(m_i, p_i)$ , i = 1, ..., n, independent, where  $p_i = \frac{1}{1 + \exp(-n_i)}$  and  $\eta_i = \beta_0 + \beta_1 x_i$ . The log-likelihood is

$$I(\beta_{0},\beta_{1}) = c + \sum_{i} \left[ y_{i} \log \frac{p_{i}}{1-p_{i}} + m_{i} \log(1-p_{i}) \right]$$

$$= c + \sum_{i} \left[ y_{i}(\beta_{0} + \beta_{1}x_{i}) - m_{i} \log(1+e^{\beta_{0}+\beta_{1}x_{i}}) \right].$$

$$\frac{1}{3} \beta_{0} = \sum_{i} y_{i} - m_{i} \frac{1}{1+e^{\beta_{0}} \beta_{1}x_{i}} \frac{1}{1+e^{\beta_{0}} \beta_{$$

### Exercise: binomial regression with a logit link

### derivation!

Then,

$$\mathcal{J}(\beta) = \begin{pmatrix} \sum_i m_i p_i (1-p_i) & \sum_i m_i x_i p_i (1-p_i) \\ \sum_i m_i x_i p_i (1-p_i) & \sum_i m_i x_i^2 p_i (1-p_i) \end{pmatrix}.$$

See my derivation in "observed\_information\_binomial\_regression.pdf".

So, since there are no y; terms left, > Expertarion don't change

$$\mathcal{I}(\beta) = \begin{pmatrix} \sum_i m_i p_i (1-p_i) & \sum_i m_i x_i p_i (1-p_i) \\ \sum_i m_i x_i p_i (1-p_i) & \sum_i m_i x_i^2 p_i (1-p_i) \end{pmatrix}.$$

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Let  $\theta^*$  denote a true value for  $\theta$ .

As  $n \to \infty$ ,

curature ( H ( I(0) ( var 6) )

$$\mathcal{I}(\boldsymbol{\theta}^*)^{1/2}(\hat{\boldsymbol{\theta}}-\boldsymbol{\theta}^*) \stackrel{\mathrm{d}}{\longrightarrow} N(0,I).$$

 $(\dot{b})$ 

That is,  $\hat{\theta} \approx^d N(\theta^*, \mathcal{I}(\theta^*)^{-1}).$ 

MIE argmax I (19)

Binomial Regression I

1107=E(-H)

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### MLE: asymptotic efficiency

- ullet Asymptotic consistency:  $\hat{m{ heta}} \stackrel{ ext{p}}{\longrightarrow} m{ heta}^*$
- Asymptotic normality:  $\hat{\theta} \approx^d N(\theta^*, \mathcal{I}(\theta^*)^{-1})$

MLE: asymptotically unbiased estimator with smallest variance  $\mathcal{I}(\theta^*)^{-1}$ .

### Wald CI for $t'\theta$ (linear combination of parameters)

use asymptotic normality

$$\boldsymbol{t} = \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_m \end{pmatrix} \qquad \boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_m \end{pmatrix} \qquad \boldsymbol{\theta}^* = \begin{pmatrix} \theta_1^* \\ \theta_2^* \\ \vdots \\ \theta_m^* \end{pmatrix} \qquad \hat{\boldsymbol{\theta}} = \begin{pmatrix} \hat{\theta}_1 \\ \hat{\theta}_2 \\ \vdots \\ \hat{\theta}_m \end{pmatrix}$$

$$\hat{\boldsymbol{\theta}} \approx N(\boldsymbol{\theta}^*, \mathcal{I}(\boldsymbol{\theta}^*)^{-1}).$$

In practice, we do not know  $\theta^*$ , the true value of  $\theta$ . Thus, we approximate  $\mathcal{I}(\theta^*)^{-1}$  using  $\mathcal{I}(\hat{\theta})^{-1}$ , leading to

$$\hat{m{ heta}} pprox \mathcal{N}(m{ heta}^*, \mathcal{I}(\hat{m{ heta}})^{-1}).$$

linear combination also follow normal distribution Then.

$$oldsymbol{t}^T\hat{oldsymbol{ heta}} pprox \mathcal{N}(oldsymbol{t}^Toldsymbol{ heta}^*,oldsymbol{t}^T\mathcal{I}(\hat{oldsymbol{ heta}})^{-1}oldsymbol{t}).$$

## Wald CI for $t^T\theta$ (linear combination of parameters)

$$\mathbf{t}^T \hat{\boldsymbol{\theta}} \approx N(\mathbf{t}^T \boldsymbol{\theta}^*, \mathbf{t}^T \mathcal{I}(\hat{\boldsymbol{\theta}})^{-1} \mathbf{t}).$$

An approximate  $100(1-\alpha)\%$  confidence interval for  $t^T\theta$ :

$$\mathbf{t}^T \hat{\boldsymbol{\theta}} \pm z_{\alpha} \sqrt{\mathbf{t}^T \mathcal{I}(\hat{\boldsymbol{\theta}})^{-1} \mathbf{t}}, \quad \text{where } \Phi(z_{\alpha}) = 1 - \alpha/2$$

In particular, taking 
$$\mathbf{t} = \text{standard unit vectors}$$
,  $\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ ,  $\begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix}$ , ...,  $\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$ , ...

we can obtain CI for each of parameters  $\theta_1, \theta_2, \dots, \theta_n$ .

An approximate 
$$100(1-\alpha)\%$$
 confidence interval for  $\theta_i$ :

$$100 > \text{ElJ}(\theta_1 \forall 1) \text{ bis when } \frac{1}{\theta_i} \pm z_{\alpha} \sqrt{(\mathcal{I}(\hat{\theta})^{-1})_{i,i}}$$

If  $\mathcal{I}$  is unavailable then we can approximate it using the observed information  $\mathcal{J}$ , i.e.,  $\mathcal{I}(\hat{\theta})^{-1} \approx \mathcal{J}(\hat{\theta}; y)^{-1}$ .

### Reminder: questions from Challenger disaster

- Forecast probability of an O-ring being damaged when the launch temperature is 29 °F.
- How good is our forecast? Can we provide a confidence interval?
- Is temperature useful to predict the O-ring failing?

How good is our forecast? Can we provide a confidence interval?

not linearly combination of J   
CI for 
$$p=g^{-1}(\eta)=rac{\exp(\eta)}{1+\exp(\eta)},$$
 where  $\eta=eta_0+eta_129.$ 

- Step 1: Compute a CI for  $\eta_r$  ( $\eta_I$ ,  $\eta_r$ ).
- Step 2: CI for  $p=g^{-1}(\eta)$  is  $(g^{-1}(\eta_I),\,g^{-1}(\eta_I))$ . Since  $g^{-1}(\eta_I)$  is unonotonic increasing function

CI for p: (0.864307, 0.9998686). See R script and result in "Confidence Interval for p" of Challenger.pdf



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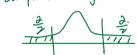
log likelihood ratio CD

 $f(x) = \frac{1}{6\sqrt{3x}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\delta}\right)^{2}}$   $\times \sim N$ 

We have

where k is the dimension of  $\theta^*$ .

This result can also, in principle, be used to construct a  $100(1-\alpha)\%$ compute non-rejection region confidence region for  $\theta$ :



 $\underbrace{\{\boldsymbol{\theta}: 2l(\hat{\boldsymbol{\theta}}) - 2l(\boldsymbol{\theta}) \leq \chi_k^2(1-\alpha)\}}_{\bullet}$ 

where  $\chi_k^2(1-\alpha)$  is the  $100(1-\alpha)\%$  point for a  $\chi_k^2$  distribution. find  $\alpha$  fall in non-rejection rejection.

This approximation is generally better than the normal approximation for  $\hat{\theta}$ . That is, it holds for smaller sample sizes.

wald CI use 2 approximation

1) normality

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log likelihood Nation OI use 1 approximate 2 I(\$1-2 I(\$4) \$\times \times \times

### MLE: regularity conditions

For maximum likelihood theory to hold we require

- $m{\theta}$  (third derivatives exist and continuous)
- Third order derivatives of I have bounded expectations
- Support of  $Y_i$  does not depend on  $\theta$
- The domain  $\Theta$  of  $\theta$  is finite dimensional and doesn't depend on  $Y_i$
- $\theta^*$  is not on the boundary of  $\Theta$ .

### References

- McCullagh & Nelder (1989), Appendix A.
- F.W. Scholz, Maximum likelihood estimation. *Encyclopedia of Statistical Sciences* Vol. 7, p.4629ff. Wiley, 2006.