Binary and binomial regression

Statistics III - CdL SSE

Tommaso Rigon
Università degli Studi di Milano-Bicocca

Homepage

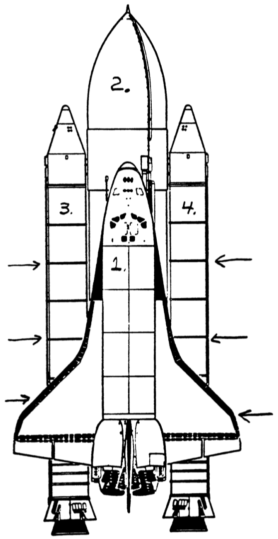


Figure 2. Space Shuttle: Orbiter, External Tank, Solid Rocket Motors, and Field Joints.

Original paper

- GLMs for **binary data** and **binomial data** are very common, whenever the response variable is dichotomous (e.g., success/failure, yes/no, dead/alive, diseased/healthy, etc.).
- This unit will cover a few additional topics related to binary and binomial regression, including:
  - grouped vs ungrouped data;
  - the choice of the link function;
  - interpretation of responses via latent “utilities”;
  - and more...
- Clearly, the most important aspects have been already covered in Unit B.

The content of this Unit is covered in **Chapter 3** of Salvan et al. (2020). Alternatively, see **Chapter 5** of Agresti (2015).

Notation and recap

- In a **binomial regression** model, we observe S_i **successes** out of m_i **trials**

$$S_i \overset{\text{ind}}{\sim} \text{Binomial}(m_i, \pi_i), \qquad g(\pi_i) = \eta_i = \boldsymbol{x}_i^T\beta, \qquad i = 1, \dots, n.$$

  We model the proportions $Y_i = S_i/m_i$, whose mean is indeed π_i and $Y_i \overset{\text{ind}}{\sim} \text{ED}(\mu_i, \mu_i(1-\mu_i)/m_i)$.

- In a **binary regression** model, we observe $Y_i \in \{0, 1\}$, which is a special case of the model above with number of trials $m_i = 1$ for all i. Thus, we have

$$Y_i \overset{\text{ind}}{\sim} \text{Bernoulli}(\pi_i), \qquad g(\pi_i) = \eta_i = \boldsymbol{x}_i^T\beta, \qquad i = 1, \dots, n.$$

In this unit, we distinguish between **two sample size measures**:

- a measure m_i for the number of Bernoulli trials that constitute a particular binomial observation;
- a measure n for the number of binomial observations.

Grouped vs ungrouped data

- If $Y_{ij} \in \{0, 1\}$ are independent **Bernoulli** random variables with success probability π_i, for $j = 1, \dots, m_i$ and $i = 1, \dots, n$, then

$$S_i = \sum_{j=1}^{m_i} Y_{ij} \sim \text{Binomial}(m_i, \pi_i).$$

- Thus, any binomial regression model can be **ungrouped** into a binary regression model with $N = \sum_{i=1}^n m_i$ observations, by simply repeating the same response and covariate m_i times.
- On the other hand, a binary regression model can be **grouped** only if multiple subjects share the same values for explanatory variables, which is common if they are all categorical.

> The **likelihood** function of these two representation **coincide** up to a proportionality constant, which means that the maximum likelihood $\hat{\beta}$ and the standard errors are identical.
>
> However, the deviance and the residuals are different, which has implications for goodness-of-fit tests and model diagnostics. The diagnostics for binary data are typically uninformative.

Link functions I

- As discussed, the **link function** is usually set to $g(\cdot) = F^{-1}(\cdot)$ for some **continuous cumulative distribution function** $F(\cdot) : \mathbb{R} \to (0, 1)$. In other words,

$$g(\pi_i) = F^{-1}(\pi_i) = \boldsymbol{x}_i^T \beta,$$

  that is

$$\mu_i = \pi_i = F(\boldsymbol{x}_i^T \beta).$$

  The function $F(\cdot)$ is monotone increasing, differentiable, and maps the real line to the unit interval.

- **Logit link**. The canonical link is the logistic link (or logit link), that is

$$g(\pi_i) = \log\left(\frac{\pi_i}{1-\pi_i}\right) = \boldsymbol{x}_i^T \beta, \qquad \text{with inverse} \qquad \pi_i = \frac{\exp(\boldsymbol{x}_i^T \beta)}{1 + \exp(\boldsymbol{x}_i^T \beta)}.$$

  Indeed, the function $F(z) = \exp(z)/(1 + \exp(z))$ with $z \in \mathbb{R}$ is the cdf of a **logistic distribution** with mean 0 and variance $\pi^2/3$.

Link functions II

- **Probit link**. The probit link is based on the standard normal cdf $\Phi(\cdot)$, i.e.

$$g(\pi_i) = \Phi^{-1}(\pi_i) = \boldsymbol{x}_i^T\beta, \qquad \text{with inverse} \qquad \pi_i = \Phi(\boldsymbol{x}_i^T\beta).$$

  The function $\Phi(z)$ with $z \in \mathbb{R}$ is usually computed numerically and equals

$$\Phi(z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right) du.$$

- **Complementary log-log link**. The complementary log-log (cloglog) link is

$$g(\pi_i) = \log(-\log(1-\pi_i)) = \boldsymbol{x}_i^T\beta, \qquad \text{with inverse} \qquad \pi_i = 1 - \exp(-\exp(\boldsymbol{x}_i^T\beta)).$$

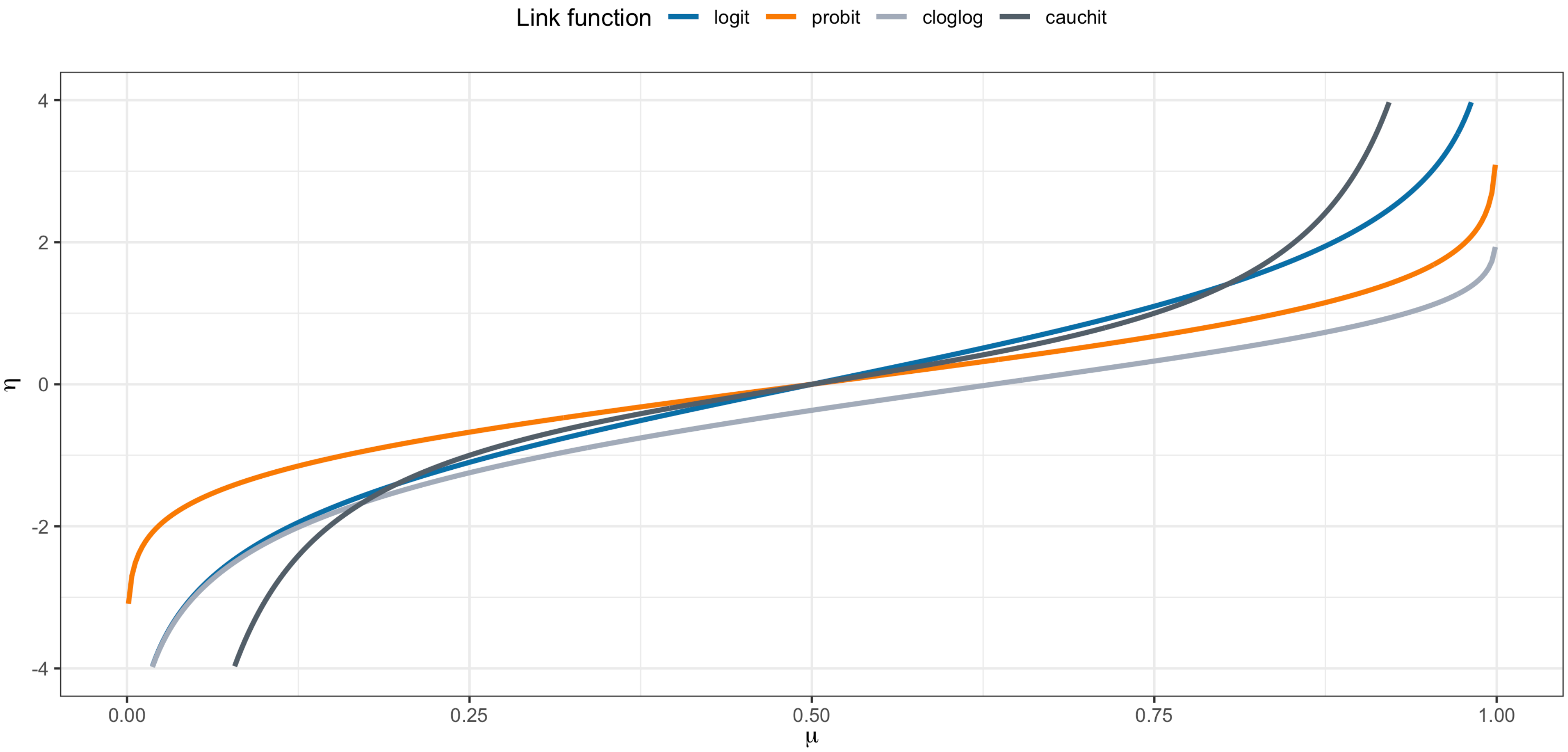
  The distribution function $F(z) = 1 - \exp(-\exp(z))$ with $z \in \mathbb{R}$ is called extreme value distribution. This link function is **asymmetric**.

- **Cauchy link**. The Cauchy link is

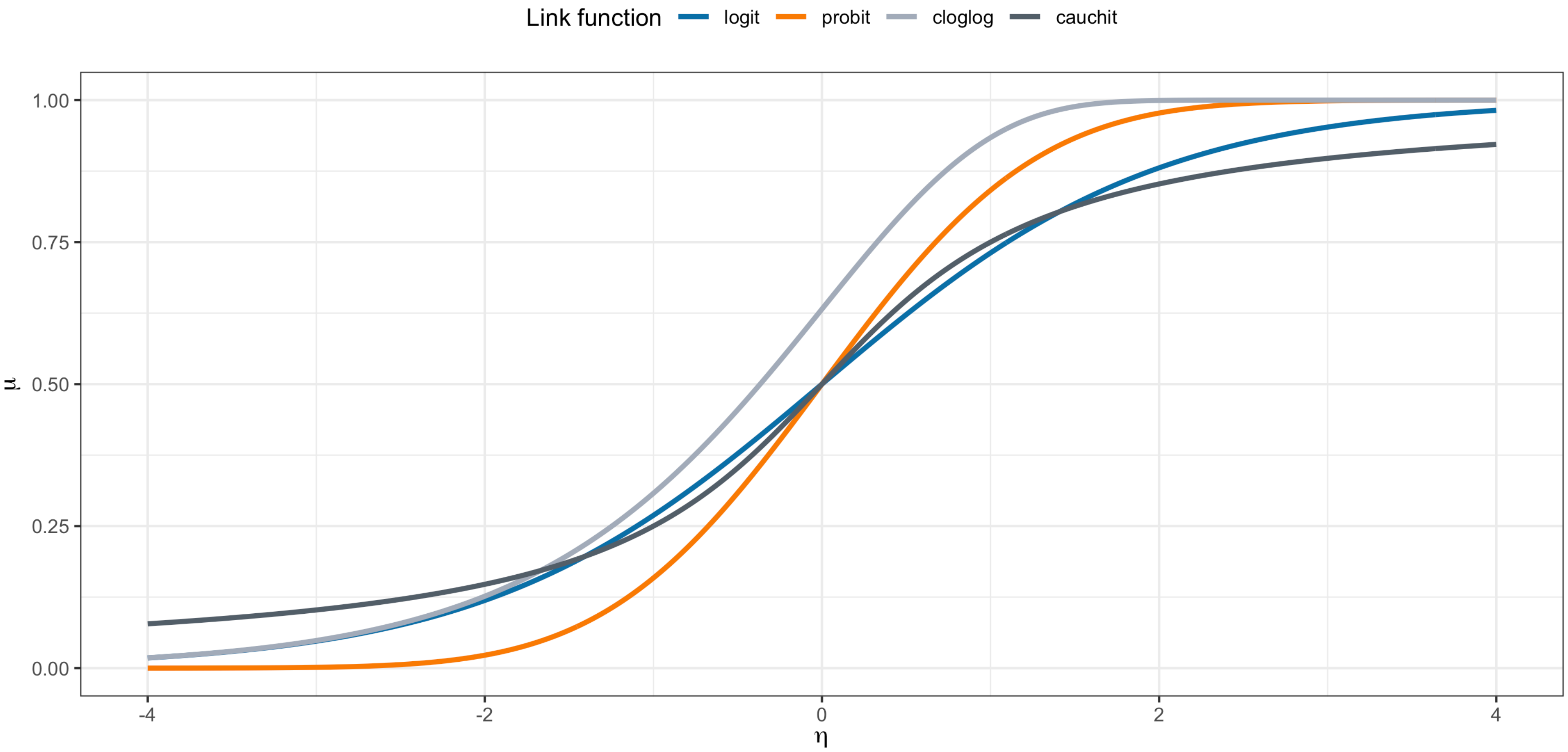
$$g(\pi_i) = \tan(\pi(\pi_i - 1/2)), \qquad \text{with inverse} \qquad \pi_i = \frac{1}{2} + \frac{\arctan(\boldsymbol{x}_i^T\beta)}{\pi}.$$

  $F(z) = 1/2 + \arctan(z)/\pi$ with $z \in \mathbb{R}$ is the cdf of a **standard Cauchy distribution**.

Link functions III



Link functions IV



Latent variable threshold models I

- A latent variable threshold model is a useful way to interpret binary regression models and choosing their link function $g(\cdot)$. Let Y_i^* be a **latent** and **continuous** random variables such that

$$Y_i^* = \boldsymbol{x}_i^T \beta + \epsilon_i, \qquad \epsilon_i \overset{\text{iid}}{\sim} F.$$

- A variable is called latent because we do not observe it directly. Instead, we observe only a **binary variable** encoding whether it exceeds a certain threshold, i.e.

$$Y_i = \mathbb{I}(Y_i^* > \tau),$$

  where $\mathbb{I}(\cdot)$ is the indicator function and τ is a threshold.

- By construction, we have $Y_i \sim \text{Bernoulli}(\pi_i)$, with

$$\pi_i = \mathbb{P}(Y_i = 1) = \mathbb{P}(Y_i^* > \tau) = \mathbb{P}(\boldsymbol{x}_i^T \beta + \epsilon_i > \tau) = 1 - \mathbb{P}(\epsilon_i \leq \tau - \boldsymbol{x}_i^T \beta) = 1 - F(\tau - \boldsymbol{x}_i^T \beta).$$

- The data contain **no information** about τ, so we can set $\tau = 0$ without loss of generality. Otherwise, the value of τ is incorporated into the intercept term.
- Likewise, an equivalent model results if we multiply all parameters by any positive constant, so we can take F to have a **standard form** with fixed variance, such as the standard normal cdf.

Latent variable threshold models II

- For most models F corresponds to a pdf that is symmetric around 0, so $F(z) = 1 - F(-z)$. Thus, we obtain

$$\pi_i = 1 - F(-\boldsymbol{x}_i^T\beta) = F(\boldsymbol{x}_i^T\beta), \qquad \text{and} \qquad F^{-1}(\pi_i) = g(\pi_i) = \boldsymbol{x}_i^T\beta.$$

That is, models for binary data naturally take the **link function** to be the **inverse of the standard cdf** for a family of continuous distributions for a latent variable.

> This dichotomization often corresponds to a real process — for instance, in medical diagnosis, preterm birth can be seen as a dichotomization of gestational age at delivery.
>
> However, there are cases where the existence of a latent quantity is more questionable, such as Y_i^* corresponding to a notion of "ability" and Y_i to "passing an exam".

Logistic regression

- The **likelihood equations** of a binomial regression model are fairly simple:

$$\sum_{i=1}^{n} \frac{m_i(y_i - \pi_i)}{\pi_i(1-\pi_i)} x_{ir} f(\eta_i) = 0, \qquad r = 1, \ldots, p,$$

where $f(z)$ is the density associated with $F(z)$, i.e. its derivative, and the **link** is $g(\cdot) = F^{-1}(\cdot)$.

- In logistic regression $f(\eta_i) = F(\eta_i)(1 - F(\eta_i)) = \pi_i(1-\pi_i)$, therefore

$$\sum_{i=1}^{n} m_i(y_i - \pi_i) x_{ir} = 0, \qquad r = 1, \ldots, p.$$

The solutions therefore has a nice interpretation as a **method of moments** estimator, in that

$$\sum_{i=1}^{n} s_i x_{ir} = \sum_{i=1}^{n} \mathbb{E}(S_i) x_{ir}, \qquad r = 1, \ldots, p,$$

Moreover, the estimated covariance matrix of $\hat{\beta}$ has a simple form:

$$\widehat{\mathrm{var}}(\hat{\beta}) = (\boldsymbol{X}^T \hat{\boldsymbol{W}} \boldsymbol{X})^{-1} = (\boldsymbol{X}^T \mathrm{diag}[m_1\hat{\pi}_1(1-\hat{\pi}_1), \ldots, m_n\hat{\pi}_n(1-\hat{\pi}_n)] \boldsymbol{X})^{-1}$$

Parameter interpretation

- We wish to **compare two estimated probabilities**, corresponding to two different covariate vectors $\boldsymbol{x} = (x_1, \dots, x_p)$ and $\boldsymbol{x}' = (x'_1, \dots, x'_p)$, namely

$$\pi(\boldsymbol{x}) = F(\boldsymbol{x}^T\beta) \qquad \text{and} \qquad \pi(\boldsymbol{x}') = F((\boldsymbol{x}')^T\beta).$$

  This is useful to understand the effect of changing covariates on the response probability.

- There are several ways to compare them, listed below, each with its advantages and disadvantages:
- The **absolute risk**, namely the difference

$$(\text{absolute risk}) = \pi(\boldsymbol{x}') - \pi(\boldsymbol{x}).$$

- The **relative risk** is the fraction

$$(\text{relative risk}) = \frac{\pi(\boldsymbol{x}')}{\pi(\boldsymbol{x})}.$$

- Both these indicators are quite interpretable but depend on the specific values of $\boldsymbol{x}$ and $\boldsymbol{x}'$, which makes it difficult to summarize the effect of a given covariate in a single number.

Odds ratio

- The **odds** is another way of summarizing probabilities, familiar to those who gamble:

$$\text{odds}(\boldsymbol{x}) = \frac{\pi(\boldsymbol{x})}{1-\pi(\boldsymbol{x})}.$$

  The odds are non-negative, with $\text{odds}(\boldsymbol{x}) > 1$ when a **success is more likely than a failure**.

- When $\pi(\boldsymbol{x}) = 0.75$ then $\text{odds}(\boldsymbol{x}) = 0.75/0.25 = 3$; a success is three times as likely as a failure. That is, we bet 3 to get 1 if we win. If instead $\text{odds}(\boldsymbol{x}) = 1/3$, we bet 1 to get 3 if we win.

- The **odds ratio** is another popular risk measure for comparing the two probabilities

$$(\text{odds ratio}) = \frac{\text{odds}(\boldsymbol{x}')}{\text{odds}(\boldsymbol{x})} = \frac{\pi(\boldsymbol{x}')}{\pi(\boldsymbol{x})} \cdot \frac{1-\pi(\boldsymbol{x})}{1-\pi(\boldsymbol{x}')}.$$

- Let $\boldsymbol{x} = (x_1, \dots, x_j, \dots, x_p)$ and $\boldsymbol{x}' = (x_1, \dots, x_j + c, \dots, x_p)$, i.e. we compare two situations in which the jth covariate is increased by a fixed amount c, then in **logistic regression**:

$$(\text{odds ratio}) = \exp(c\beta_j),$$

  which is a **constant number** that does not depend on $\boldsymbol{x}$. This is not true e.g. in probit.

Odds ratio and logistic regression

- Let $\boldsymbol{x}$ be a generic covariate vector and consider its odds under a **logistic regression** model:

$$\text{odds}(\boldsymbol{x}) = \frac{\pi(\boldsymbol{x})}{1-\pi(\boldsymbol{x})} = \frac{\exp(\boldsymbol{x}^T\beta)}{1+\exp(\boldsymbol{x}^T\beta)} \cdot \left(\frac{1}{1+\exp(\boldsymbol{x}^T\beta)}\right)^{-1} = \exp(\boldsymbol{x}^T\beta).$$

  Thus, the odds of any predicted value is simply the exponential of the linear predictor $\boldsymbol{x}^T\beta$.

- Consequently, in general the **odds ratio** is

$$(\text{odds ratio}) = \frac{\text{odds}(\boldsymbol{x}')}{\text{odds}(\boldsymbol{x})} = \exp\{(\boldsymbol{x}' - \boldsymbol{x})^T\beta\}$$

- If the only change is in the jth covariate, from x_j to $x_j + c$, then the odds ratio becomes

$$(\text{odds ratio}) = \exp\{(\boldsymbol{x}' - \boldsymbol{x})^T\beta\} = \exp(c\beta_j).$$

  In particular, $\exp(\beta_j)$ represents the odds ratio after a **unitary increase** of the jth covariate.

Residuals and diagnostics for binary data

- In presence of **binary data**, namely when $m_i = 1$ and $Y_i \sim \text{Bernoulli}(\pi_i)$, many the diagnostic tools are **degenerate** and uninformative.
- For example, the `fitted` vs `residuals` plot, namely the dispersion plot of the points $(\hat{\pi}_i, y_i - \hat{\pi}_i)$, simply shows two parallel lines with slope -1, which is uninformative.
- As an extreme case, consider the **null model** in which $\pi_1 = \cdots = \pi_n$, then the X^2 statistic is

$$X^2 = \sum_{i=1}^{n} \frac{(y_i - \hat{\pi})^2}{\hat{\pi}(1-\hat{\pi})} = n.$$

- A common solution is to **group the data** according to some criteria, although this introduces approximations and some arbitrariness (i.e. the Hosmer-Lemeshow test).
- In terms of prediction, there exists various indices and techniques that you will cover in Data Mining. The simplest index is the **accuracy**, i.e. the fraction of correct predictions.

Overdispersion

- In binomial regression the main **assumption** is that $S_i \sim \text{Binomial}(m_i, \pi_i)$, implying that

$$\text{var}(Y_i) = \frac{\pi_i(1-\pi_i)}{m_i},$$

where implicitly we have set $\phi = 1$.

- However, from the analysis of the residuals or by computing the X^2 statistic we may realize that the data present **overdispersion**, namely the **correct model** is such that

$$\text{var}(Y_i) = \phi \frac{\pi_i(1-\pi_i)}{m_i},$$

with $\phi > 1$. This implies that the binomial regression model is **misspecified**.

- The two most common solutions to overdispersion are the following:

  i. the usage of **quasi-likelihoods**;

  ii. using another parametric distribution, beyond the class of exponential dispersion families; a typical choice is the **beta-binomial**.

References

Agresti, A. (2015), *Foundations of Linear and Generalized Linear Models*, Wiley.

Salvan, A., Sartori, N., and Pace, L. (2020), *Modelli lineari generalizzati*, Springer.