Generalized Linear Models

Statistics III - CdL SSE

Tommaso Rigon
Università degli Studi di Milano-Bicocca

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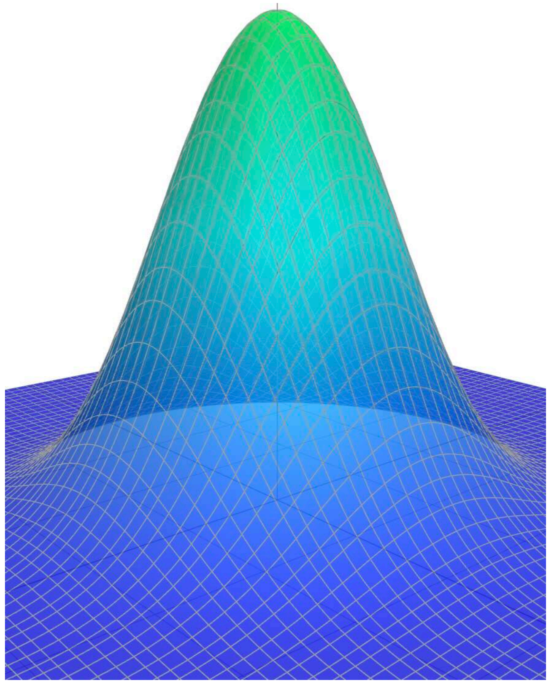


- This unit will cover the following **topics**:
  - Exponential dispersion families
  - Likelihood, inference, and testing
  - Iteratively Re-weighted Least Squares (IRLS)
  - Deviance, model checking, and residuals
  - Model selection
- GLMs are regression models with a linear predictor, where the response variable follows an **exponential dispersion family**.
- The symbol 📖 means that a few extra steps are discussed in the **handwritten notes**.

The content of this Unit is covered in **Chapter 2** of Salvan et al. (2020). Alternatively, see **Chapter 4** of Agresti (2015) or **Chapter 6** of Azzalini (2008).

Introduction

Preliminaries

- GLMs are a **class** of **regression models** in which a **response** random variable Y_i is modeled as a function of a vector of **covariates** $\boldsymbol{x}_i \in \mathbb{R}^p$.
- The random variables Y_i are not restricted to be Gaussian. For example:
  - $Y_i \in \{0, 1\}$, known as **binary regression**
  - $Y_i \in \{0, 1, \dots\}$, known as **count regression**
  - $Y_i \in (0, \infty)$ or $Y_i \in (-\infty, \infty)$
- Gaussian linear models are a special case of GLMs, arising when $Y_i \in (-\infty, \infty)$.

- The **response random variables** are collected in the random vector $\boldsymbol{Y} = (Y_1, \dots, Y_n)^T$, whose **observed realization** is $\boldsymbol{y} = (y_1, \dots, y_n)^T$.
- The **design matrix** $\boldsymbol{X}$ is an $n \times p$ **non-stochastic** matrix containing the covariate values. The jth variable (column) is denoted by $\tilde{\boldsymbol{x}}_j$, while the ith observation (row) is $\boldsymbol{x}_i$.
- We assume that $\boldsymbol{X}$ has **full rank**, that is, $\text{rk}(\boldsymbol{X}) = p$ with $p \leq n$.

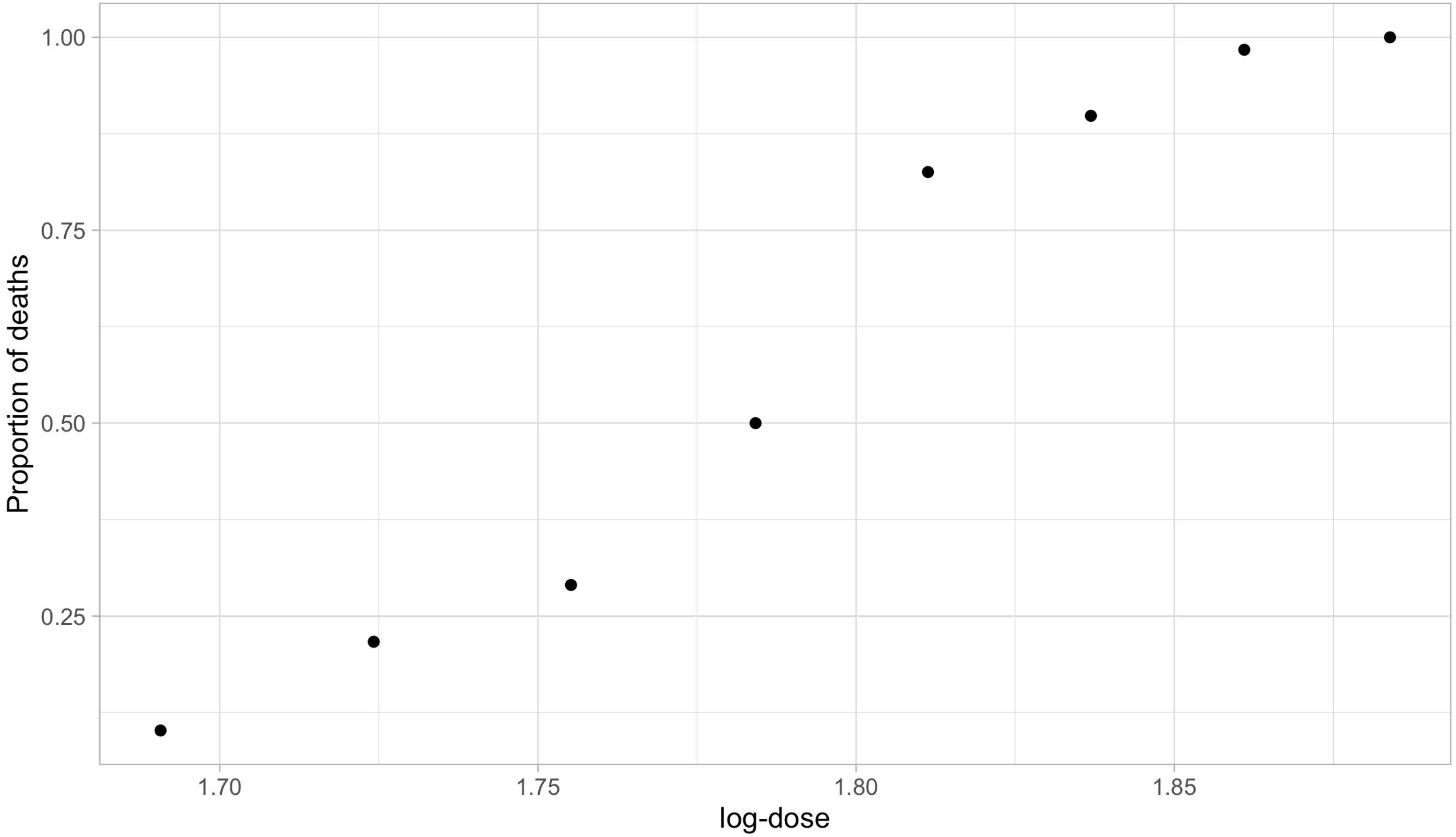
Beetles data, from Bliss (1935)

- The Beetles dataset originates from Bliss (1935). It records the number of adult flour beetles that died after a 5-hour exposure to gaseous carbon disulphide.

m	deaths	logdose
59	6	1.6907
60	13	1.7242
62	18	1.7552
56	28	1.7842
63	52	1.8113
59	53	1.8369
62	61	1.8610
60	60	1.8839

- We aim to predict the proportion of deaths as a function of logdose.
- Modeling death proportions directly with **linear models** is **inappropriate**. A **variable transformation** provides a more **principled** solution, but it comes with **drawbacks**.

Beetles data, a dose-response plot



- There is a clear **positive** and **non-linear** pattern between the **proportion of deaths** as a function of the logdose. The response variable take values in $[0, 1]$.

Modelling the Beetles data

- Let S_i be the number of dead beetles out of m_i, and let x_i denote the log-dose. By definition, $S_i \in \{0, 1, \dots, m_i\}$ for $i = 1, \dots, 8$.
- It is natural to model each S_i as **independent binomial** random variables, counting the number of deaths out of m_i individuals. In other words:

$$S_i \overset{\text{ind}}{\sim} \text{Binomial}(m_i, \pi_i), \qquad i = 1, \dots, 8,$$

  where π_i is the **probability** of death at a given dose x_i. Moreover, et $Y_i = S_i/m_i$ be the proportion of deaths, then:

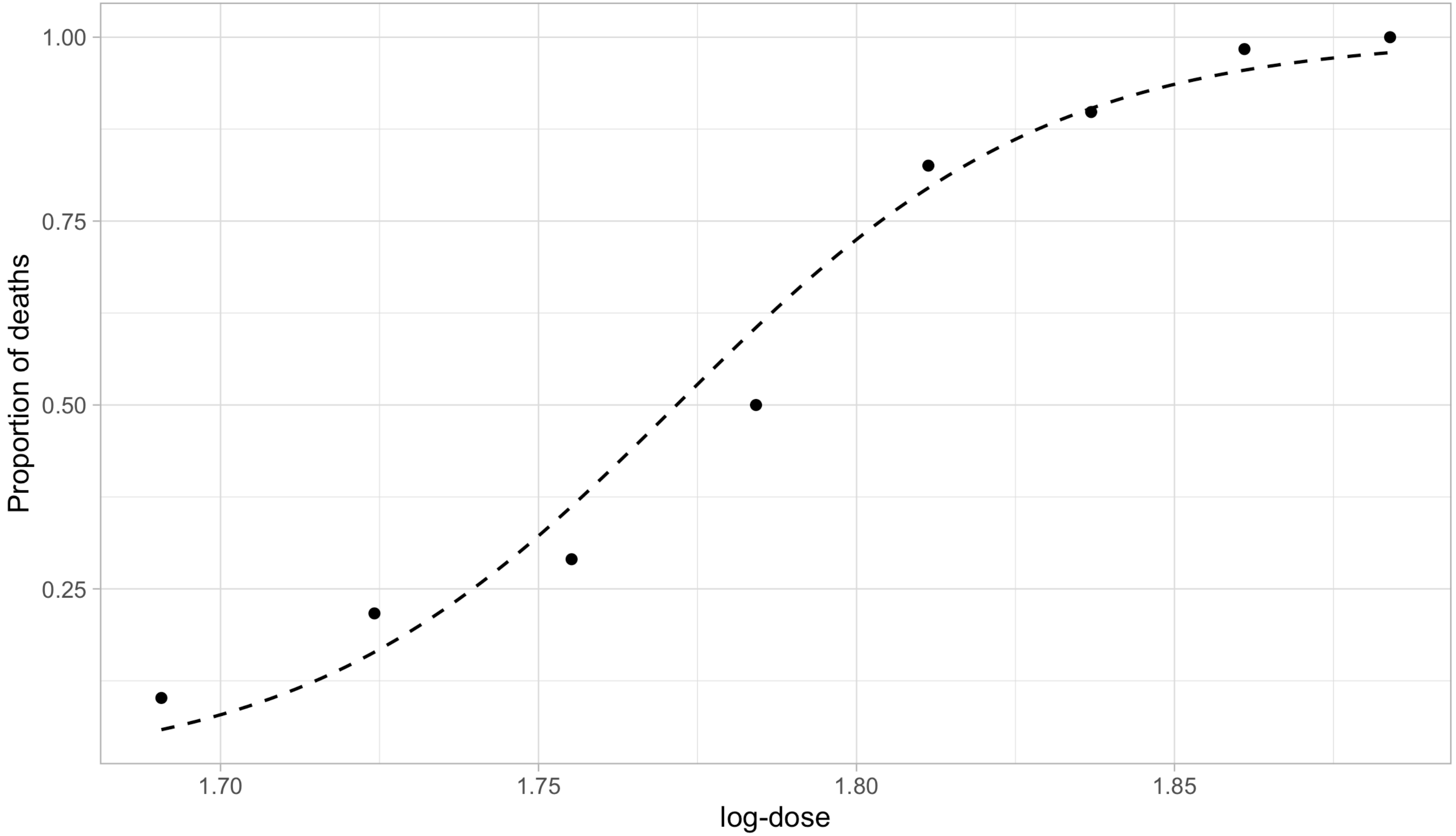
$$\mathbb{E}(Y_i) = \mathbb{E}\left(\frac{S_i}{m_i}\right) = \pi_i = \mu_i.$$

- A modeling approach, called **logistic regression**, specifies:

$$g(\pi_i) = \log\left(\frac{\pi_i}{1 - \pi_i}\right) = \beta_1 + \beta_2 x_i \quad \Longrightarrow \quad \pi_i = g^{-1}(\beta_1 + \beta_2 x_i) = \frac{\exp(\beta_1 + \beta_2 x_i)}{1 + \exp(\beta_1 + \beta_2 x_i)}.$$

  for some parameters $\beta_1, \beta_2 \in \mathbb{R}$. **Note** that $\pi_i \in (0, 1)$ by construction.

Beetles data, fitted model



- The **maximum likelihood** estimates are $\hat{\beta}_1 = -60.72$ and $\hat{\beta}_2 = 34.3$. This yields the **predictive curve** $\hat{\pi}(x) = g^{-1}(\hat{\beta}_1 + \hat{\beta}_2 x)$, which estimates the mean proportion $\mathbb{E}(S_i/m_i)$.

A comparison with old tools I

Let $Y_i = S_i/m_i$ be the proportion of deaths. A direct application of linear models implies:

$$Y_i = \beta_1 + \beta_2 x_i + \epsilon_i.$$

The coefficients β_1 and β_2 are then estimated using OLS using Y_i as response.

- The prediction $\hat{\beta}_1 + \hat{\beta}_2 x_i$ is **unrestricted**, meaning it could produce values like “1.3” or “-2” as estimated **proportions**, which is clearly undesirable.
- The **additive structure** $Y_i = \beta_1 + \beta_2 x_i + \epsilon_i$ cannot hold with **iid** errors ϵ_i, because S_i, and thus Y_i, are **discrete**. As a result, the errors are always **heteroschedastic**.
- If $m_i = 1$, i.e. when the data are **binary**, all the above issues are **exacerbated**.

This approach is sometimes called the **linear probability model**. Before GLMs, it was considered acceptable despite its issues, but by modern standards it should **not be used**.

A comparison with old tools II

We consider the **empirical logit** variable transformation of $Y_i = S_i/m_i$, obtaining

$$\text{logit}(\tilde{Y}_i) = \log\left(\frac{S_i + 0.5}{m_i - S_i + 0.5}\right) = \beta_1 + \beta_2 x_i + \epsilon_i, \qquad \tilde{Y}_i = \frac{S_i + 0.5}{m_i + 1}.$$

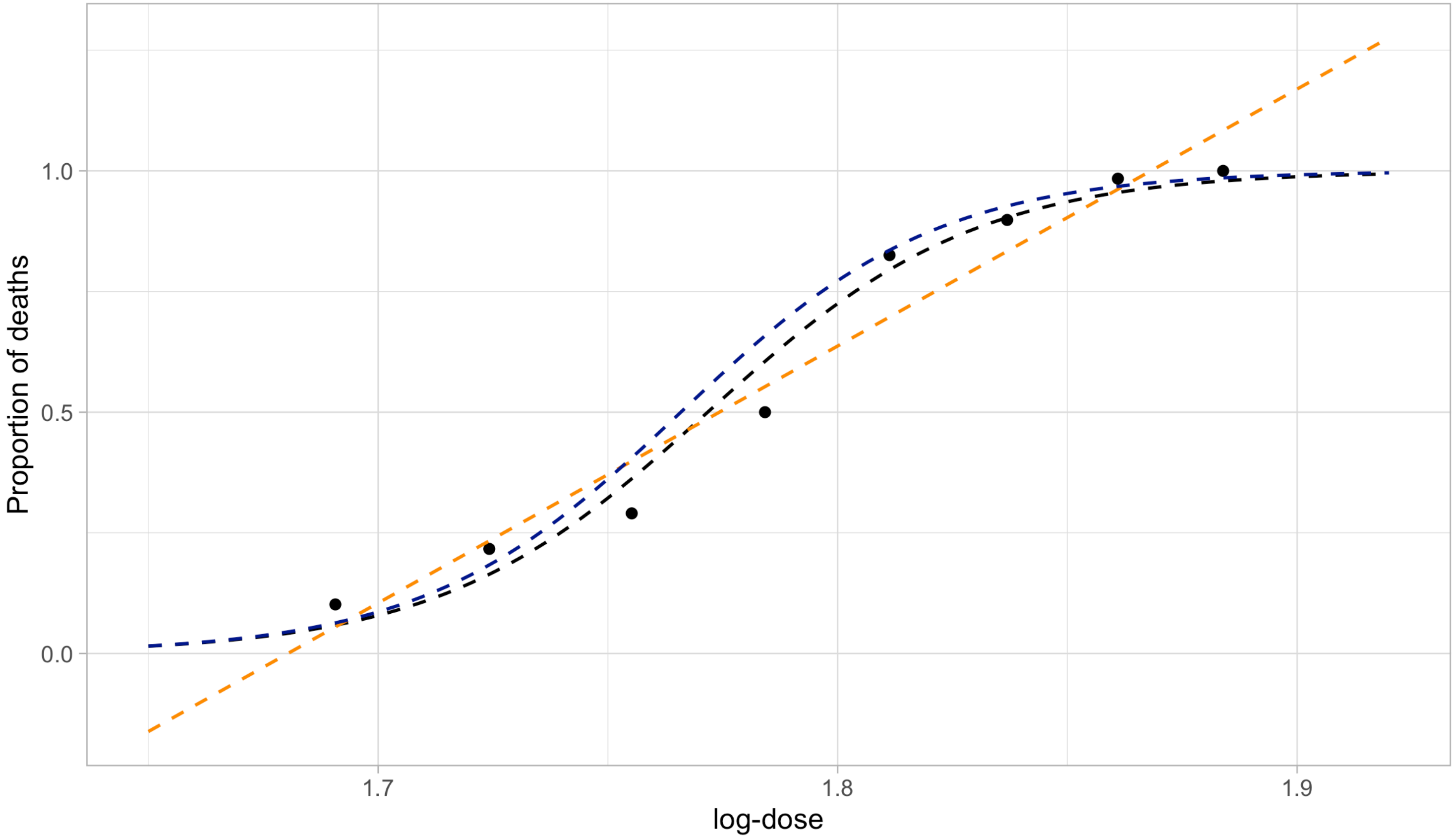
A correction term is necessary because otherwise $g(\cdot) = \text{logit}(\cdot)$ is undefined. The predictions belong to $(0,1)$, since

$$\hat{\pi}_i = g^{-1}[\mathbb{E}\{g(\tilde{Y}_i)\}] = g^{-1}(\hat{\beta}_1 + \hat{\beta}_2 x_i) = \frac{\exp(\hat{\beta}_1 + \hat{\beta}_2 x_i)}{1 + \exp(\hat{\beta}_1 + \hat{\beta}_2 x_i)},$$

in which $\hat{\beta}_1$ and $\hat{\beta}_2$ are estimated with OLS using $\text{logit}(\tilde{Z}_i)$ as response.

- The **interpretation** of $\hat{\beta}$ is less clear, as they refer to the mean of $\text{logit}(\tilde{Y}_i)$ instead of $\mathbb{E}(Y_i)$.
- An arbitrary **boundary correction** is needed.
- Inference is problematic and requires further corrections, because of **heteroschedastic** errors.
- This approach is **not compatible** with the reasonable assumption $S_i \sim \text{Binomial}(m_i, \pi_i)$.

A comparison with old tools III



- The black line is the predicted curve of a **logistic regression GLM**. The orange line is the predictived curve of a **linear model**. The blue line is the predictive curve of a **linear model** after an **empirical logit variable transformation**.

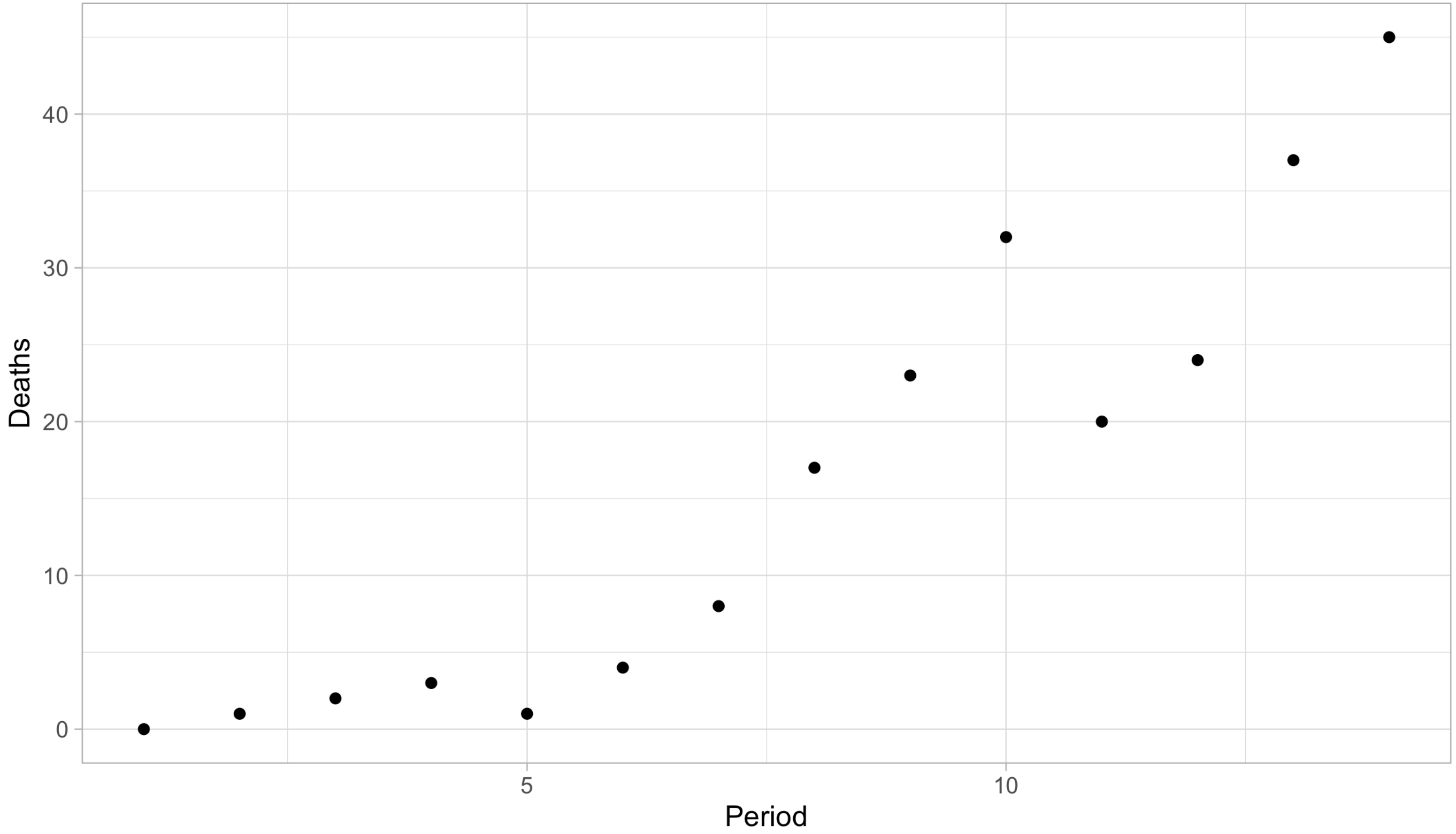
Aids data

- Number of AIDS deaths in Australia in a sequence of three-months periods between 1983 and 1986.

	1983-1	**1984-1**	**1985-1**	**1986-1**	**1983-2**	**1984-2**	**1985-2**	**1986-2**	**1983-3**	**1984-3**	**1985-3**	**1986-3**	**1983-4**	**1984-4**
deaths	0	1	2	3	1	4	8	17	23	32	20	24	37	45
period	1	2	3	4	5	6	7	8	9	10	11	12	13	14

- We are interested in predicting the number of deaths as a function of the period of time.
- The response variable $Y_i \in \{0, 1, \dots\}$ is a non-negative **count**.

Aids data, scatter plot



- There is a clear positive association between period and deaths. However, the increase appears to be **faster** than **linear**. Note that both the mean and the **variability** of Y_i increase over time.

Modelling the Aids data

- Let Y_i be the number of deaths, and let x_i denote the period. By definition, $Y_i \in \{0, 1, \dots\}$ are non-negative counts, for $i = 1, \dots, 14$.

- We model Y_i as **independent Poisson** random variables, counting the number of deaths:

$$Y_i \overset{\text{ind}}{\sim} \text{Poisson}(\mu_i), \qquad i = 1, \dots, 14,$$

  where μ_i is the **mean** of Y_i, namely $\mathbb{E}(Y_i) = \mu_i$.

- A modeling approach, called **Poisson regression**, specifies:

$$g(\mu_i) = \log(\mu_i) = \beta_1 + \beta_2 x_i \quad \Longrightarrow \quad \mu_i = g^{-1}(\beta_1 + \beta_2 x_i) = \exp(\beta_1 + \beta_2 x_i),$$

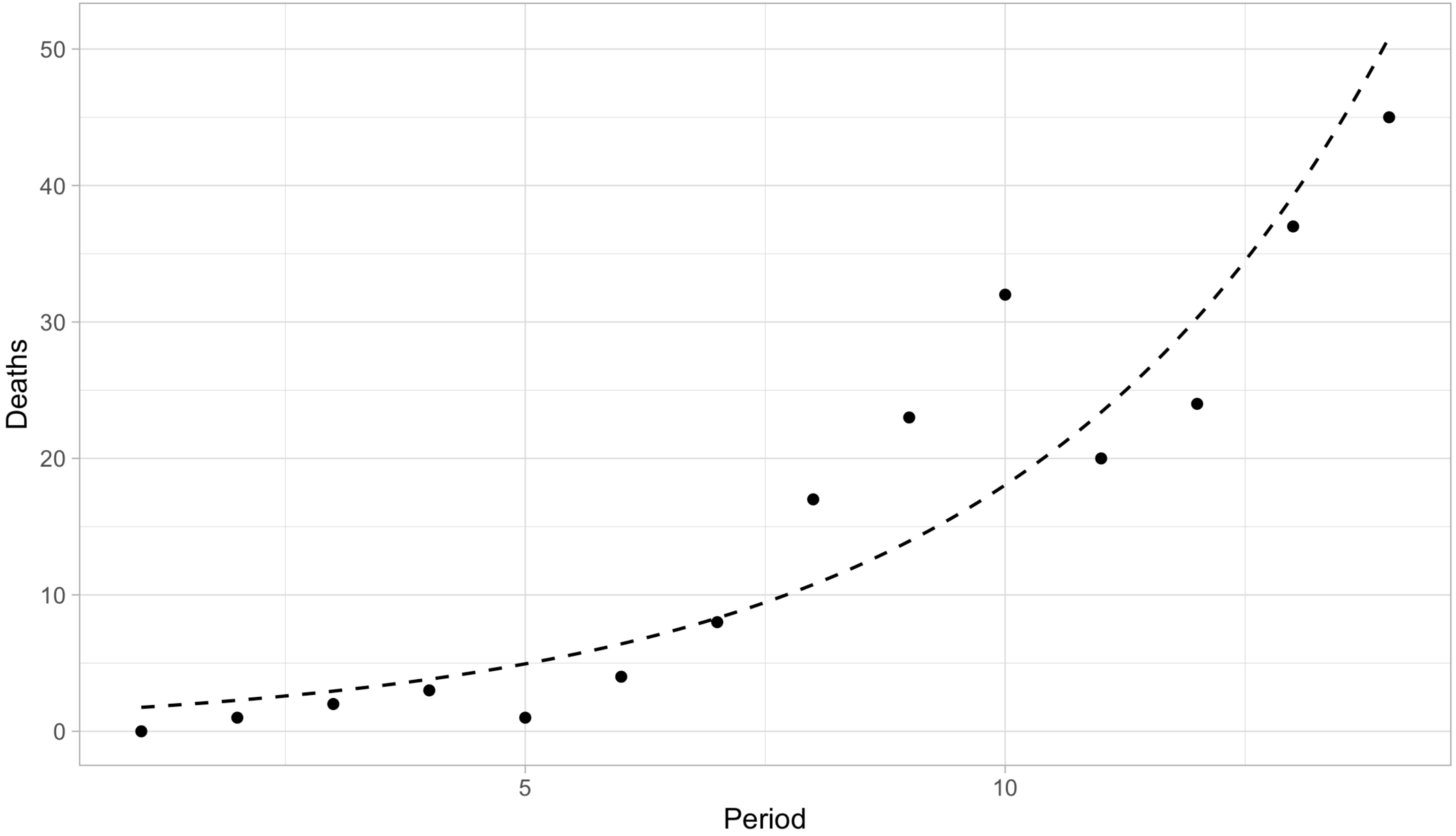
  for some parameters $\beta_1, \beta_2 \in \mathbb{R}$. **Note** that $\mu_i > 0$ by construction.

- Under this specification, the **variances** of the observations are

$$\text{var}(Y_i) = \mu_i = \exp(\beta_1 + \beta_2 x_i),$$

  which increases with x, as desired. This implies that $Y_1, \dots, Y_n$ are **heteroschedastic**, but this is not an issue in GLMs, as this aspect is **automatically accounted** for.

Aids data, fitted model



- The **maximum likelihood** estimates are $\hat{\beta}_1 = 0.304$ and $\hat{\beta}_2 = 0.259$. This yields the **predictive curve** $\hat{\mu}(x) = \exp(\hat{\beta}_1 + \hat{\beta}_2 x)$, which estimates the mean $\mathbb{E}(Y_i)$.

A comparison with old tools I

We consider the **variance-stabilizing** transformation $S_i = \sqrt{Y_i}$, obtaining

$$\sqrt{Y_i} = \beta_1 + \beta_2 x_i + \epsilon_i.$$

The predictions belong to $(0, \infty)$, since

$$\hat{\mu}_i = \mathbb{E}(\sqrt{Y_i})^2 = (\hat{\beta}_1 + \hat{\beta}_2 x_i)^2,$$

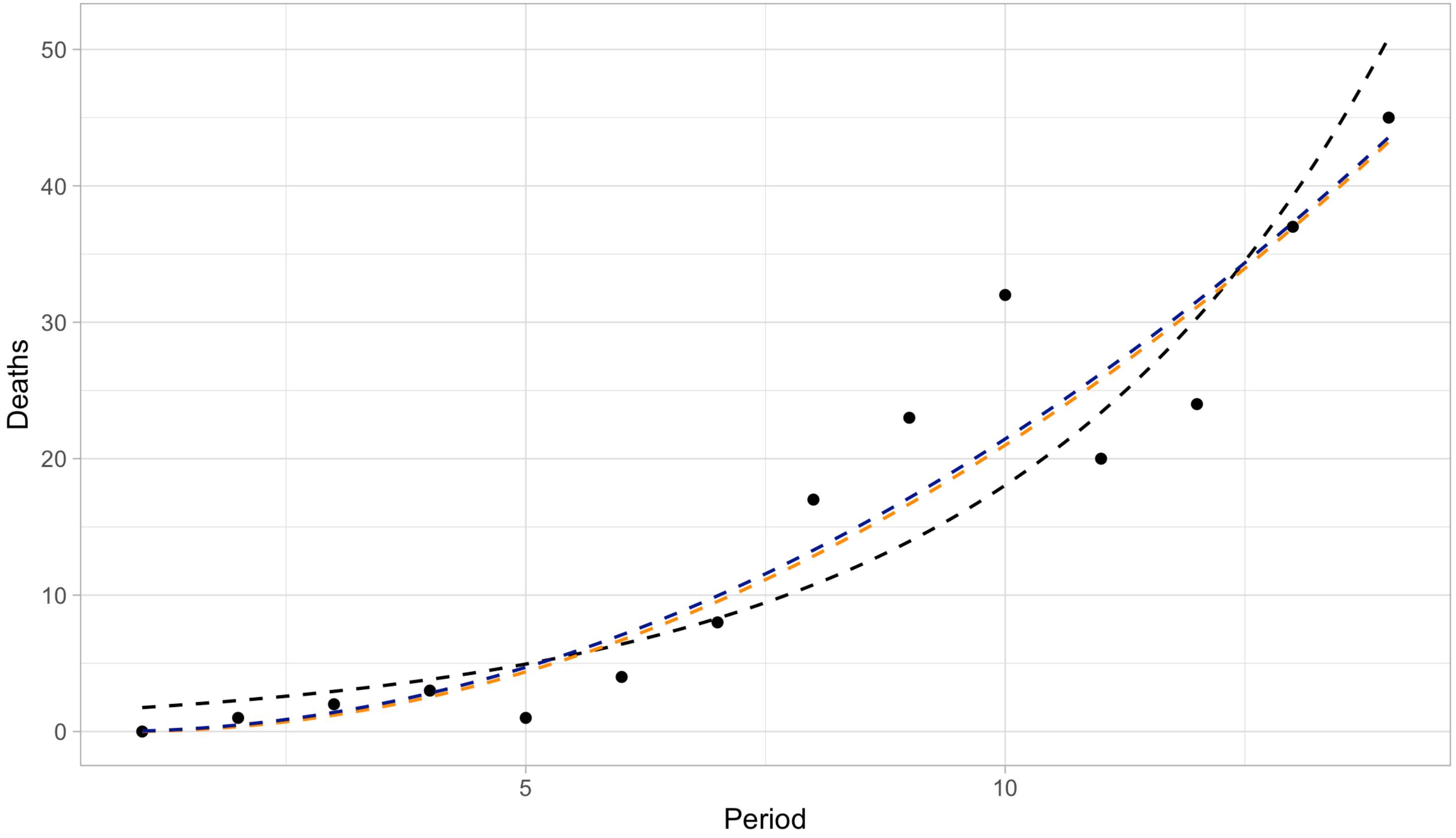
in which $\hat{\beta}_1$ and $\hat{\beta}_2$ are estimated with OLS using $\sqrt{Y_i}$ as response.

- The **interpretation** of $\hat{\beta}$ is less clear, as they refer to the mean of $\sqrt{Y}_i$ instead of $\mathbb{E}(Y_i)$.
- This approach is **not compatible** with the reasonable assumption $Y_i \sim \text{Poisson}(\mu_i)$ and it only valid as an **asymptotic approximation**.

To compare such a model with a similar specification, we also fit another Poisson GLM in which

$$Y_i \overset{\text{ind}}{\sim} \text{Poisson}(\mu_i), \qquad \sqrt{\mu_i} = \beta_1 + \beta_2 x_i, \qquad i = 1, \dots, 14.$$

A comparison with old tools II



- The black line is the predicted curve of a **Poisson regression GLM** with logarithmic link. The orange line is the predicted curve of a **linear model** with a **square-root transformation**. The blue line is the predictive curve of a **Poisson regression GLM** with **square-root link**.

The components of a GLM

- **Random component**. This specifies the probability distribution response variable Y_i. The observations $\boldsymbol{y} = (y_1, \dots, y_n)$ on that distribution are treated as **independent**.

- **Linear predictor**. For a parameter vector $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)^T$ and an $n \times p$ design matrix $\boldsymbol{X}$, the linear predictor is $\boldsymbol{\eta} = \boldsymbol{X}\beta$. We will also write

$$\eta_i = \boldsymbol{x}_i^T\beta = x_{i1}\beta_1 + \cdots + x_{ip}\beta_p, \qquad i = 1, \dots, n.$$

- **Link function**. This is an invertible and differentiable function $g(\cdot)$ applied to each component of the **mean** $\mu_i = \mathbb{E}(Y_i)$ that relates it to the linear predictor:

$$g(\mu_i) = \eta_i = \boldsymbol{x}_i^T\beta, \qquad \Longrightarrow \qquad \mu_i = g^{-1}(\eta_i) = g^{-1}(\boldsymbol{x}_i^T\beta).$$

> Note that, in general, we **cannot** express the response in an additive way $Y_i = g^{-1}(\eta_i) + \epsilon_i$.

Random component of a GLM

- In GLMs the random variables Y_i are **independent** and they are distributed according to an **exponential dispersion family**, whose definition will be provided in a few slides.
- The **distributions most commonly** used in Statistics, such as the normal, binomial, gamma, and Poisson, are exponential family distributions.
- Exponential dispersion families are **characterized** by their **mean** and **variance**. Let $v(\mu) > 0$ be a function of the mean, called **variance function** and let $a_i(\phi) > 0$ be functions of an additional unknown parameter $\phi > 0$ called **dispersion**.

In a GLMs the observations are independent draws from a distribution $\mathrm{ED}(\mu_i, a_i(\phi)v(\mu_i))$:

$$Y_i \overset{\text{ind}}{\sim} \mathrm{ED}(\mu_i, a_i(\phi)v(\mu_i)), \qquad \mathbb{E}(Y_i) = \mu_i, \qquad g(\mu_i) = \boldsymbol{x}_i^T\beta,$$

with $\mu_i \in \mathcal{M}$. Moreover, the **variance** is connected to the **mean** via $v(\mu)$:

$$\mathrm{var}(Y_i) = a_i(\phi)v(\mu_i),$$

where $a_i(\phi) = \phi/\omega_i$ and ω_i are **known weights**. Special cases are $a_i(\phi) = \phi$ and $a_i(\phi) = 1$.

Notable examples

In a **Gaussian linear model** we consider the **identity link** $g(\mu) = \mu$ and let

$$Y_i \overset{\text{ind}}{\sim} \mathrm{N}(\mu_i, \sigma^2), \qquad \mu_i = \boldsymbol{x}_i^T \beta.$$

The unknown variance $\sigma^2 = \phi$ is called **dispersion** in GLMs. The **parameter space** is $\mathcal{M} = \mathbb{R}$, whereas $a_i(\phi) = \phi$ and the variance function is **constant** $v(\mu) = 1$ (homoschedasticity).

In a **binomial regression model** with **logit link** $g(\mu) = \mathrm{logit}(\mu)$ we let $Y_i = S_i/m_i$ and

$$S_i \overset{\text{ind}}{\sim} \mathrm{Binomial}(m_i, \pi_i), \qquad \mathbb{E}\,(Y_i) = \pi_i = \mu_i, \qquad \mathrm{logit}(\mu_i) = \boldsymbol{x}_i^T \beta.$$

We have $a_i(\phi) = 1/m_i$ and $v(\mu) = \mu(1-\mu)$. There is **no dispersion** parameter.

In **Poisson regression** with **logarithmic link** $g(\mu) = \log(\mu)$ we let

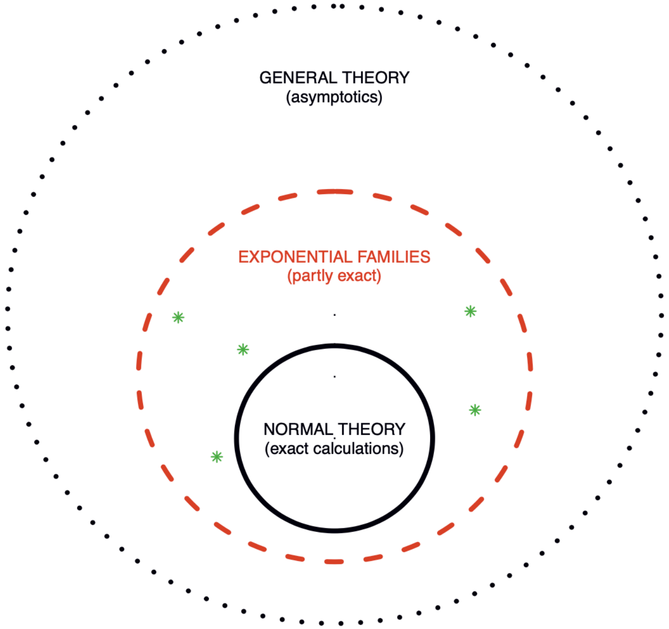
$$Y_i \overset{\text{ind}}{\sim} \mathrm{Poisson}(\mu), \qquad \log(\mu_i) = \boldsymbol{x}_i^T \beta.$$

We have $a_i(\phi) = 1$ and $v(\mu) = \mu$. There is **no dispersion** parameter.

Exponential dispersion families

Overview

- Figure 1 of Efron (2023). **Three level** of statistical modeling.



- The **prime role** of **exponential families** in the theory of statistical inference was first emphasized by Fisher (1934).
- Most **well-known distributions**—such as Gaussian, Poisson, Binomial, and Gamma—are instances of exponential families.

Exponential dispersion family: definition

The **density** of Y_i belongs to an **exponential dispersion family** if it can be written as

$$p(y_i; \theta_i, \phi) = \exp\left\{\frac{\theta_i y_i - b(\theta_i)}{a_i(\phi)} + c(y_i, \phi)\right\},$$

where $y_i \in \mathcal{Y} \subseteq \mathbb{R}$, $\theta_i \in \Theta \subseteq \mathbb{R}$ and $a_i(\phi) = \phi/\omega_i$ where ω_i are **known positive weights**. The parameter θ_i is called **natural parameter** while ϕ is called **dispersion** parameter.

- By specifying the functions $a_i(\cdot), b(\cdot)$ and $c(\cdot)$ one obtain a particular **parametric model**.
- The support $\mathcal{Y}$ of Y_i does not depend on the parameters ϕ or θ_i and $b(\cdot)$ can be **differentiated** infinitely many times. In particular, this is a **regular statistical model**.
- As mentioned, special cases are $a_i(\phi) = \phi$ and $a_i(\phi) = 1$. When $a_i(\phi) = 1$ and $c(y_i, \phi) = c(y_i)$ we obtain

$$p(y_i; \theta_i) = \exp\left\{\theta_i y_i - b(\theta_i) + c(y_i)\right\},$$

which is called **natural exponential family** of order 1.

Mean and variance I 📖

- Let us consider the **log-likelihood** contribution of the ith observations, which is defined as

$$\ell(\theta_i, \phi; y_i) = \log p(y_i; \theta_i, \phi) = \frac{\theta_i y_i - b(\theta_i)}{a_i(\phi)} + c(y_i, \phi).$$

  If you prefer, this is the log-likelihood when the sample size $n = 1$ and we only observe Y_i.

- The **score** and **hessian** functions, namely the first and second derivative over θ_i are

$$\frac{\partial}{\partial \theta_i}\ell(\theta_i, \phi; y_i) = \frac{y_i - b'(\theta_i)}{a_i(\phi)}, \qquad \frac{\partial^2}{\partial \theta_i^2}\ell(\theta_i, \phi; y_i) = \frac{-b''(\theta_i)}{a_i(\phi)}.$$

  where $b'(\cdot)$ and $b''(\cdot)$ denote the **first** and **second** derivative of $b(\cdot)$.

- Recall the following **Bartlett identities**, valid in any **regular** statistical model:

$$\mathbb{E}\left(\frac{\partial}{\partial \theta_i}\ell(\theta_i, \phi; Y_i)\right) = 0,$$

$$\mathbb{E}\left\{\left(\frac{\partial}{\partial \theta_i}\ell(\theta_i, \phi; Y_i)\right)^2\right\} = \text{var}\left(\frac{\partial}{\partial \theta_i}\ell(\theta_i, \phi; Y_i)\right) = \mathbb{E}\left(-\frac{\partial^2}{\partial \theta_i^2}\ell(\theta_i, \phi; Y_i)\right).$$

Mean and variance II 📖

- Specializing Bartlett identities in **exponential dispersion families**, we obtain

$$\mathbb{E}\left(\frac{Y_i - b'(\theta_i)}{a_i(\phi)}\right) = 0, \qquad \text{var}\left(\frac{Y_i - b'(\theta_i)}{a_i(\phi)}\right) = \frac{\text{var}(Y_i)}{a_i(\phi)^2} = \frac{b''(\theta_i)}{a_i(\phi)}.$$

Re-arranging the terms, we finally get the following key result.

> Let Y_i be an exponential dispersion family, identified by the functions $a_i(\cdot), b(\cdot)$ and $c(\cdot)$, and with natural parameter θ_i. Then the **mean** and the **variance** of Y_i equal
>
> $$\mathbb{E}(Y_i) = b'(\theta_i), \qquad \text{var}(Y_i) = a_i(\phi)b''(\theta_i).$$

- The mean $\mu_i = b'(\theta_i)$ does **not** depend on the **dispersion** parameter.
- We have $b''(\cdot) > 0$ because $\text{var}(Y_i)$, which means that $b(\cdot)$ is a **convex function**.
- Moreover, the function $b'(\theta)$ is **continuous** and **monotone increasing** and hence **invertible**.

The function $b(\cdot)$ is related to the moment generating function of Y_i. Thus, higher order derivatives of $b(\cdot)$ allows the calculations of skewness, kurtosis, etc.

Mean parametrization, variance function

Let Y_i be an exponential dispersion family, identified by the functions $a_i(\cdot), b(\cdot)$ and $c(\cdot)$, and with **natural parameter** θ_i, then

$$\mu(\theta_i) := \mu_i = \mathbb{E}(Y_i) = b'(\theta_i).$$

The function $\mu(\cdot) : \Theta \to \mathcal{M}$ is **one-to-one** and invertible, that is, a **reparametrization** of θ_i. We call μ_i the **mean parametrization** of an exponential dispersion family.

- The **inverse** relationship, re-obtaining θ_i as a function of μ_i, is denoted with

$$\theta_i = \theta(\mu_i) = b'^{-1}(\mu_i).$$

- Using this notation, we can express the variance of Y_i as a function of μ_i as follows

$$\text{var}(Y_i) = a_i(\phi)b''(\theta_i) = a_i(\phi)b''(\theta(\mu_i)) = a_i(\phi)v(\mu_i),$$

  where $v(\mu_i) := b''(\theta(\mu_i))$ is the **variance function**.

- The domain $\mathcal{M}$ and the variance function $v(\mu)$ **characterize** the function $b(\cdot)$ and the entire distribution, for any given $a_i(\phi)$. This justifies the **notation** $Y_i \sim \text{ED}(\mu_i, a_i(\phi)v(\mu_i))$.

Gaussian distribution 📖

- Let $Y_i \sim \mathrm{N}(\mu_i, \sigma^2)$. The **density** function of Y_i can be written as

$$
\begin{aligned}
p(y_i; \mu_i, \sigma^2) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(y_i - \mu_i)^2\right\} \\
&= \exp\left\{\frac{y_i\mu_i - \mu_i^2/2}{\sigma^2} - \frac{\log(2\pi\sigma^2)}{2} - \frac{y_i^2}{2\sigma^2}\right\}
\end{aligned}
$$

- Then, we can recognize the following relationships:

$$
\theta_i = \theta(\mu_i) = \mu_i, \quad a_i(\phi) = \phi = \sigma^2, \quad b(\theta_i) = \frac{\theta_i^2}{2}, \quad c(y_i, \phi) = -\frac{\log(2\pi\phi)}{2} - \frac{y_i^2}{2\phi}.
$$

  In the Gaussian case, the **mean parametrization** and the **natural parametrization** coincide. Moreover, the **dispersion** ϕ coincides with the **variance** σ^2.

- Using the results we previously discussed, we obtain the well-known relationships

$$
\mathbb{E}(Y_i) = b'(\theta_i) = \theta_i, \qquad \mathrm{var}(Y_i) = a_i(\phi)b''(\theta_i) = \phi.
$$

  The **variance function** $v(\mu_i) = 1$ is **constant**. We will write $Y_i \sim \mathrm{ED}(\mu_i, \phi)$ with $\mu_i \in \mathcal{M} = \mathbb{R}$.

Poisson distribution 📖

Let $Y_i \sim \text{Poisson}(\mu_i)$. The **pdf** function of Y_i can be written as

$$\begin{aligned} p(y_i; \mu_i) = \frac{\mu_i^{y_i} e^{-\mu_i}}{y_i!} &= \exp\{y_i \log(\mu_i) - \mu_i - \log(y_i!)\} \\ &= \exp\{y_i\theta_i - e^{\theta_i} - \log(y_i!)\}, \qquad y_i = 0, 1, 2, \dots . \end{aligned}$$

- Then, we can recognize the following relationships:

$$\begin{aligned} \theta_i &= \theta(\mu_i) = \log(\mu_i), & a_i(\phi) &= 1, \\ b(\theta_i) &= e^{\theta_i}, & c(y_i, \phi) &= c(y_i) = -\log(y_i!). \end{aligned}$$

  There is **no dispersion** parameter since $a_i(\phi) = 1$.

- Using the results we previously discussed, we obtain the well-known relationships

$$\begin{aligned} \mathbb{E}(Y_i) &= b'(\theta_i) = e^{\theta_i} = \mu_i, \\ \text{var}(Y_i) &= a_i(\phi)b''(\theta_i) = e^{\theta_i} = \mu_i. \end{aligned}$$

  The **variance function** $v(\mu_i) = \mu_i$ is **linear**. We will write $Y_i \sim \text{ED}(\mu_i, \mu_i)$ with $\mu_i \in (0, \infty)$.

Gamma distribution I 📖

- Let $Y_i \sim \text{Gamma}(\alpha, \lambda_i)$. The **density** function of Y_i can be written as

$$\begin{aligned} p(y_i; \alpha, \lambda_i) &= \frac{\lambda_i^{\alpha} y_i^{\alpha-1} e^{-\lambda_i y_i}}{\Gamma(\alpha)} \\ &= \exp\left\{\alpha \log \lambda_i - \lambda_i y_i + (\alpha - 1)\log y_i - \log \Gamma(\alpha)\right\} \\ &= \exp\left\{\alpha\left(\log \lambda_i - \frac{\lambda_i}{\alpha} y_i\right) + (\alpha - 1)\log y_i - \log \Gamma(\alpha)\right\} \\ &= \exp\left\{\frac{\theta_i y_i + \log(-\theta_i)}{\phi} - (1/\phi)\log \phi + (1/\phi - 1)\log y_i - \log \Gamma(1/\phi)\right\}, \qquad y > 0, \end{aligned}$$

  having defined the **dispersion** $\phi = 1/\alpha$ and the **natural parameter** $\theta_i = -\lambda_i/\alpha$.

- Then, we can recognize the following relationships:

$$a_i(\phi) = \phi, \qquad b(\theta_i) = -\log(-\theta_i),$$
$$c(y_i, \phi) = -(1/\phi)\log \phi + (1/\phi - 1)\log y_i - \log \Gamma(1/\phi).$$

Gamma distribution II 📖

- Using the results we previously discussed, we obtain the well-known relationships

$$\mathbb{E}(Y_i) = b'(\theta_i) = -\frac{1}{\theta_i} = \frac{\alpha}{\lambda_i} = \mu_i, \qquad \text{var}(Y_i) = a_i(\phi)b''(\theta_i) = \frac{\phi}{\theta_i^2} = \frac{\alpha}{\lambda_i^2}.$$

- At the same time, we can write the **inverse** relationship linking θ_i to the **mean** as

$$\theta_i = \theta(\mu_i) = -\frac{1}{\mu_i}$$

  from which we finally obtain the following **quadratic** variance function

$$v(\mu_i) = \mu_i^2.$$

- We will write $Y_i \sim \text{ED}(\mu_i, \phi\mu_i^2)$ with $\mu_i \in (0, \infty)$.

Binomial distribution I 📖

- Let $S_i \sim \text{Binomial}(m_i, \pi_i)$, with $\pi_i \in (0,1)$. The random variable $Y_i = S_i/m_i$ has **density**

$$
\begin{aligned}
p(y_i; m_i, \pi_i) &= \binom{m_i}{m_i y_i} \pi_i^{m_i y_i} (1-\pi_i)^{m_i - m_i y_i} \\
&= \binom{m_i}{m_i y_i} \left(\frac{\pi_i}{1-\pi_i}\right)^{m_i y_i} (1-\pi_i)^{m_i} \\
&= \exp\left\{ m_i y_i \log\left(\frac{\pi_i}{1-\pi_i}\right) + m_i \log(1-\pi_i) + \log\binom{m_i}{m_i y_i} \right\},
\end{aligned}
$$

for $y_i \in \{0, 1/m_i, 2/m_2, \dots, m_i/m_i\}$. This can be written as

$$
p(y_i; m_i, \pi_i) = \exp\left\{ \frac{y_i\theta_i - \log\{1+\exp(\theta_i)\}}{1/m_i} + \log\binom{m_i}{m_i y_i} \right\},
$$

where the **natural parameter** is $\theta_i = \text{logit}(\pi_i) = \log\{\pi/(1-\pi_i)\}$.

Binomial distribution II 📖

- Note that $\mathbb{E}(Y_i) = \mathbb{E}(Z_i/m_i) = \pi_i = \mu_i$. This means there **no dispersion** parameter ϕ and

$$\theta_i = \text{logit}(\mu_i), \quad a_i(\phi) = \frac{1}{m_i}, \quad b(\theta_i) = \log\{1 + \exp(\theta_i)\}, \quad c(y_i) = \log\binom{m_i}{m_i y_i}.$$

- Using the general formulas therefore we obtain

$$\begin{aligned}\mathbb{E}(Y_i) &= b'(\theta_i) = \frac{\exp(\theta_i)}{1 + \exp(\theta_i)} = \mu_i, \\ \text{var}(Y_i) &= a_i(\phi) b''(\theta_i) = \frac{1}{m_i}\frac{\exp(\theta_i)}{[1 + \exp(\theta_i)]^2} = \frac{\mu_i(1-\mu_i)}{m_i},\end{aligned}$$

  from which we obtain that the **variance function** is $v(\mu_i) = \mu_i(1-\mu_i)$ is quadratic.

- We will write $Y_i \sim \text{ED}(\mu_i, \mu_i(1-\mu_i)/m_i)$ with $\mu_i \in \mathcal{M} = (0,1)$.

Notable exponential dispersion families

Model	$\mathrm{N}(\mu_i, \sigma^2)$	$\mathrm{Gamma}(\alpha, \alpha/\mu_i)$	$\frac{1}{m_i}\mathrm{Binomial}(m_i, \mu_i)$	$\mathrm{Poisson}(\mu_i)$
Support $\mathcal{Y}$	$\mathbb{R}$	$[0, \infty)$	$\{0, 1/m_i, \dots, 1\}$	$\mathbb{N}$
$\theta_i = \theta(\mu_i)$	μ_i	$-1/\mu_i$	$\log\left(\frac{\mu_i}{1-\mu_i}\right)$	$\log \mu_i$
Parametric space Θ	$\mathbb{R}$	$(-\infty, 0)$	$\mathbb{R}$	$\mathbb{R}$
$b(\theta_i)$	$\theta_i^2/2$	$-\log(-\theta_i)$	$\log\{1 + \exp(\theta_i)\}$	$\exp(\theta_i)$
ϕ	σ^2	$1/\alpha$	1	1
$a_i(\phi)$	σ^2	$1/\alpha$	$1/m_i$	1
$\mathcal{M}$	$\mathbb{R}$	$(0, \infty)$	$(0, 1)$	$(0, \infty)$
$v(\mu_i)$	1	μ_i^2	$\mu_i(1 - \mu_i)$	μ_i

> The list of exponential dispersion families does not end here. Other examples are the **inverse Gaussian**, the **negative binomial** and **hyperbolic secant** distributions.

Link functions and canonical link

- To complete the GLM specification, we need to choose a **link function** $g(\cdot)$ such that:

$$g(\mu_i) = \boldsymbol{x}_i^T \beta, \qquad \theta_i = \theta(\mu_i) \quad \Longrightarrow \quad \theta_i = \theta(g^{-1}(\boldsymbol{x}_i^T \beta)).$$

- It is fairly natural to consider a **monotone** and **differentiable** link function $g(\cdot) : \mathcal{M} \to \mathbb{R}$ so that the inverse $g^{-1}(\cdot) : \mathbb{R} \to \mathcal{M}$. This ensures that the predictions are well-defined.

$$\mathbb{E}(Y_i) = g^{-1}(\boldsymbol{x}_i^T \beta) \in \mathcal{M}.$$

- For example, in **binary regression** any continuous **cumulative distribution function** for $g^{-1}(\cdot)$ leads to a good link function, such as $g(\cdot) = \Phi(\cdot)$ (probit) or $g^{-1}(\eta_i) = e^{\eta_i}/(1 + e^{\eta_i})$ (logistic).

The following link is called **canonical link** and it is implied by the distribution:

$$g(\mu_i) = \theta(\mu_i) \quad \Longrightarrow \quad \theta_i = \boldsymbol{x}_i^T \beta.$$

- The **identity** link is canonical for the **Gaussian**, the **logarithm** is canonical for the **Poisson**, the **logit** is canonical for the Binomial and the **reciprocal** is canonical for the **Gamma**.

Likelihood quantities

Likelihood function

- Let $Y_i \overset{\text{ind}}{\sim} \text{ED}(\mu_i, a_i(\phi)v(\mu_i))$ be the response variable of a GLM, with $g(\mu_i) = \boldsymbol{x}_i^T\beta$. The **joint distribution** of the responses $\boldsymbol{Y} = (Y_1, \dots, Y_n)$ is

$$p(\boldsymbol{y}; \beta, \phi) = \prod_{i=1}^n p(y_i; \beta, \phi) = \prod_{i=1}^n \exp\left\{\frac{y_i\theta_i - b(\theta_i)}{a_i(\phi)} + c(y_i, \phi)\right\}.$$

  with $\theta_i = \theta(\mu_i) = \theta(g^{-1}(\boldsymbol{x}_i^T\beta))$.

- The **log-likelihood** function therefore is

$$\ell(\beta, \phi) = \sum_{i=1}^n \frac{y_i\theta_i - b(\theta_i)}{a_i(\phi)} + c(y_i, \phi).$$

- In general, there is **no sufficient statistic** with dimension smaller than n.

Likelihood equations I 📖

- To conduct inference using the **classical theory** (as in *Statistica II*), we need to consider the first and second derivative of the log-likelihood, that is, the **score function**

$$\ell_*(\beta;\phi) := \frac{\partial}{\partial\beta}\ell(\beta,\phi),$$

and the **observed information matrix** $\boldsymbol{J}$, whose elements are

$$j_{rs} = -\frac{\partial}{\partial\beta_r}\frac{\partial}{\partial\beta_s}\ell(\beta,\phi), \qquad r,s = 1,\dots,p.$$

- These quantities have a **simple expression** in the end, but getting there requires quite a **bit of calculus**.

> Let us focus on the estimation of β, assuming for now that ϕ is a **known parameter**, as is the case in binomial or Poisson regression.
>
> This assumption is not restrictive, even when ϕ is actually unknown. In fact, we will show that the maximum likelihood estimate $\hat{\beta}$ does not depend on ϕ, and that β and ϕ are **orthogonal**.

Likelihood equations II 📖

- Let us begin by noting that

$$\ell_r(\beta;\phi) = \frac{\partial}{\partial \beta_r}\ell(\beta,\phi) = \sum_{i=1}^n \frac{1}{a_i(\phi)}\left(y_i\frac{\partial \theta_i}{\partial \beta_r} - \frac{\partial b(\theta_i)}{\partial \beta_r}\right), \qquad r = 1,\dots,p.$$

Such an expression can be **simplified** because

$$\frac{\partial b(\theta_i)}{\partial \beta_r} = b'(\theta_i)\frac{\partial \theta_i}{\partial \beta_r} = \mu_i\frac{\partial \theta_i}{\partial \beta_r},$$

which implies that the score function will have the following **structure**:

$$\frac{\partial}{\partial \beta_r}\ell(\beta,\phi) = \sum_{i=1}^n \frac{1}{a_i(\phi)}(y_i - \mu_i)\frac{\partial \theta_i}{\partial \beta_r}, \qquad r = 1,\dots,p.$$

- Recall that $a_i(\phi) = \phi/\omega_i$, hence the **maximum likelihood estimator** is obtained by solving:

$$\cancel{\frac{1}{\phi}}\sum_{i=1}^n \omega_i(y_i - \mu_i)\frac{\partial \theta_i}{\partial \beta_r} = 0, \qquad r = 1,\dots,p.$$

Likelihood equations III 📖

> Let $f(x)$ be a function with **inverse** $g(x) = f^{-1}(x)$ and **first derivative** $f'(x)$. Then
>
> $$\frac{\partial g}{\partial x} = [f^{-1}]'(x) = \frac{1}{f'(f^{-1}(x))}.$$

- Recall that $g(\mu_i) = \boldsymbol{x}_i^T\beta = \eta_i$ and that $\theta_i = \theta(\mu_i)$ is the inverse of $\mu(\theta_i)$. As an **application** of the above **lemma**:

  $$\frac{\partial \theta_i}{\partial \mu_i} = \theta'(\mu_i) = \frac{1}{\mu'(\theta(\mu_i))} = \frac{1}{b''(\theta(\mu_i))} = \frac{1}{v(\mu_i)},$$

  Moreover, since we $\mu_i = g^{-1}(\eta_i)$ we obtain

  $$\frac{\partial \mu_i}{\partial \eta_i} = \frac{1}{g'(g^{-1}(\eta_i))} = \frac{1}{g'(\mu_i)}.$$

- Summing up, the **chain rule of derivation** for **composite functions** gives:

  $$\frac{\partial \theta_i}{\partial \beta_r} = \frac{\partial \theta_i}{\partial \mu_i}\frac{\partial \mu_i}{\partial \eta_i}\frac{\partial \eta_i}{\partial \beta_r} = \frac{1}{v(\mu_i)}\frac{1}{g'(\mu_i)}x_{ir}, \qquad r = 1, \dots, p.$$

Likelihood equations IV 📖

- Combining all the above equations, we obtain an explicit formula for the **score function**

$$\frac{\partial}{\partial \beta_r}\ell(\beta,\phi) = \frac{1}{\phi}\sum_{i=1}^n \omega_i \frac{(y_i-\mu_i)}{v(\mu_i)}\frac{x_{ir}}{g'(\mu_i)} = \sum_{i=1}^n \frac{(y_i-\mu_i)}{\mathrm{var}(Y_i)}\frac{x_{ir}}{g'(\mu_i)}, \qquad r=1,\dots,p.$$

The **maximum likelihood estimator** solves the **likelihood equations**:

$$\sum_{i=1}^n \omega_i \frac{(y_i-\mu_i)}{v(\mu_i)}\frac{x_{ir}}{g'(\mu_i)} = 0, \qquad r=1,\dots,p,$$

which **do not depend** on ϕ. In **matrix notation**

$$\boldsymbol{D}^T\boldsymbol{V}^{-1}(\boldsymbol{y}-\boldsymbol{\mu}) = \boldsymbol{0},$$

where $\boldsymbol{V} = \mathrm{diag}(v(\mu_1)/\omega_1,\dots,v(\mu_n)/\omega_n)$ and $\boldsymbol{D}$ is an $n \times p$ matrix whose elements are

$$d_{ir} = \frac{\partial \mu_i}{\partial \beta_r} = \frac{\partial \mu_i}{\partial \eta_i}\frac{\partial \eta_i}{\partial \beta_r} = \frac{1}{g'(\mu_i)}x_{ir}, \qquad i=1,\dots,n, \quad r=1,\dots,p.$$

Canonical link: simplifications 📖

- When using the **canonical link** $\theta(\mu_i) = g(\mu_i)$ significant simplifications arise, because

$$\frac{\partial \theta_i}{\partial \mu_i} = \frac{1}{v(\mu_i)} = g'(\mu_i) \quad \Longrightarrow \quad v(\mu_i)g'(\mu_i) = 1.$$

Thus, plugging-in this equality in the former equations, gives:

$$\frac{\partial \theta_i}{\partial \beta_r} = x_{ir}, \qquad r = 1, \dots, p,$$

which is not surprising, because the canonical link implies $\theta_i = x_{i1}\beta_1 + \cdots + x_{ip}\beta_p$.

The **likelihood equations** under the **canonical link** are

$$\sum_{i=1}^{n} \omega_i (y_i - \mu_i) x_{ir} = 0, \qquad r = 1, \dots, p.$$

Let $\boldsymbol{\Omega} = \text{diag}(\omega_1, \dots, \omega_n)$, then in **matrix notation** we have $\boldsymbol{X}^T\boldsymbol{\Omega}(\boldsymbol{y} - \boldsymbol{\mu}) = \boldsymbol{0}$. The equations simplify even further when the weights are constant, i.e. $\boldsymbol{\Omega} = I_n$, yielding $\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{\mu}) = \boldsymbol{0}$.

Examples of estimating equations

Let $Y_i \sim \mathrm{ED}(\mu_i, \phi)$ with $g(\mu_i) = \mu_i$, namely the **Gaussian** linear model with the **identity** (canonical) link. The likelihood equations are

$$\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{X}\beta) = \boldsymbol{0},$$

which are also called **normal equations**. Their solution over β is the OLS $\hat{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$.

Let $Y_i \sim \mathrm{ED}(\mu_i, \phi/\omega_i)$ with $g(\mu_i) = \mu_i$, namely the **Gaussian** linear model with the **identity** (canonical) link and **heteroschedastic errors**. The likelihood equations are

$$\boldsymbol{X}^T\boldsymbol{\Omega}(\boldsymbol{y} - \boldsymbol{X}\beta) = \boldsymbol{0},$$

Their solution over β is the weighted least square estimator $\hat{\beta}_{\text{wls}} = (\boldsymbol{X}^T\boldsymbol{\Omega}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Omega}\boldsymbol{y}$.

Let $Y_i \sim \mathrm{ED}(\mu_i, \mu_i)$ with $g(\mu_i) = \log\mu_i$, namely a **Poisson** regression model with the **logarithmic** (canonical) link. The likelihood equations can be solved **numerically**

$$\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{\mu}) = \boldsymbol{0}, \qquad \boldsymbol{\mu} = (e^{\boldsymbol{x}_1^T\beta}, \dots, e^{\boldsymbol{x}_n^T\beta}).$$

Example: Beetles data

- Using the Beetles data, we specified a **binomial logistic** regression model for the counts $m_i Y_i \sim \text{Binomial}(m_i, \pi_i)$ with mean $\mathbb{E}(Y_i) = \pi_i = \exp(\beta_1 + \beta_2 x_i)/(1 + \exp(\beta_1 + \beta_2 x_i))$.
- The **maximum likelihood estimate** $(\hat{\beta}_1, \hat{\beta}_2)$ is the value solving simultaneously:

$$\sum_{i=1}^n m_i y_i = \sum_{i=1}^n m_i \frac{\exp(\beta_1 + \beta_2 x_i)}{1 + \exp(\beta_1 + \beta_2 x_i)}, \quad \text{and} \quad \sum_{i=1}^n m_i x_i y_i = \sum_{i=1}^n m_i x_i \frac{\exp(\beta_1 + \beta_2 x_i)}{1 + \exp(\beta_1 + \beta_2 x_i)}.$$

  Unfortunately, there is **no closed form** solution.
- In our case, we have that

$$\sum_{i=1}^n m_i y_i = 291, \qquad \sum_{i=1}^n m_i x_i y_i = 532.2083.$$

- With these values, we can use the **numerical** algorithm IRLS to solve the above system, obtaining

$$\hat{\beta} = (\hat{\beta}_1, \hat{\beta}_2) = (-60.717, 34.270).$$

Example: Beetles data

- The **predicted response** can be computed by using the formula

$$\hat{\mu}_i = \frac{\exp(\hat{\beta}_1 + \hat{\beta}_2 x_i)}{1 + \exp(\hat{\beta}_1 + \hat{\beta}_2 x_i)} = \frac{\exp(-60.717 + 34.270 x_i)}{1 + \exp(-60.717 + 34.270 x_i)}, \qquad i = 1, \dots, 8.$$

m_i	deaths (S_i)	logdose (x_i)	$Y_i = S_i/m_i$	$\hat{\mu}_i$
59	6	1.691	0.102	0.059
60	13	1.724	0.217	0.164
62	18	1.755	0.290	0.362
56	28	1.784	0.500	0.605
63	52	1.811	0.825	0.795
59	53	1.837	0.898	0.903
62	61	1.861	0.984	0.955
60	60	1.884	1.000	0.979

- The predicted values and the data Y_i were also shown in a **plot** at the beginning of this unit.

Example: Aids data

- In the Aids data, we specified a **Poisson** regression model with $\mathbb{E}(Y_i) = \exp(\beta_1 + \beta_2 x_i)$.
- The maximum likelihood estimate $(\hat{\beta}_1, \hat{\beta}_2)$ **solve** simultaneously:

$$\sum_{i=1}^n y_i = \sum_{i=1}^n \exp(\beta_1 + \beta_2 x_i), \quad \text{and} \quad \sum_{i=1}^n x_i y_i = \sum_{i=1}^n x_i \exp(\beta_1 + \beta_2 x_i).$$

- This system does **not** always admits a **solution**. This happens, for example, in the **extreme case** $\sum_{i=1}^n y_i = 0$, occurring when all counts equal zero.

- Using the Aids data we have $\sum_{i=1}^n y_i = 217$ and $\sum_{i=1}^n x_i y_i = 2387$. Via **numerical methods** we solve the above system of equations and we obtain $\hat{\beta}_1 = 0.304$ and $\hat{\beta}_2 = 0.259$.
- The estimated mean values are $\hat{\mu}_i = \exp(0.304 + 0.259 x_i)$ and in particular the mean for the **next period** is

$$\hat{\mu}_{i+1} = \exp(0.304 + 0.259(x_i + 1)) = \exp(0.259)\hat{\mu}_i = 1.296\hat{\mu}_i.$$

In other words, the estimated number of deaths increases by about 30% every trimester.

Example: Aids data

	deaths (Y_i)	period (x_i)	$\hat{\mu}_i$
1983-1	0	1	1.755
1984-1	1	2	2.274
1985-1	2	3	2.946
1986-1	3	4	3.817
1983-2	1	5	4.945
1984-2	4	6	6.407
1985-2	8	7	8.301
1986-2	17	8	10.755
1983-3	23	9	13.934
1984-3	32	10	18.052
1985-3	20	11	23.389
1986-3	24	12	30.302
1983-4	37	13	39.259
1984-4	45	14	50.863

- The predicted values and the data Y_i were also shown in a **plot** at the beginning of this unit.

Observed and expected information I 📖

- Let us first consider the negative derivative of the score function, that is the **observed information matrix** $\boldsymbol{J}$ with entries:

$$j_{rs} = -\frac{\partial}{\partial \beta_s}\left[\frac{\partial}{\partial \beta_r}\ell(\beta,\phi)\right] = -\frac{\partial}{\partial \beta_s}\sum_{i=1}^n \frac{1}{a_i(\phi)}(y_i - \mu_i)\frac{\partial \theta_i}{\partial \beta_r}$$
$$= \sum_{i=1}^n \frac{1}{a_i(\phi)}\left[\frac{\partial \mu_i}{\partial \beta_s}\frac{\partial \theta_i}{\partial \beta_r} - (y_i - \mu_i)\frac{\partial^2 \theta_i}{\partial \beta_r \partial \beta_s}\right], \qquad r,s = 1,\dots,p.$$

- Let $\boldsymbol{I} = \mathbb{E}(\boldsymbol{J})$ be the $p \times p$ **Fisher information matrix** associated with β, whose elements are

$$i_{rs} = \mathbb{E}(j_{rs}) = \mathbb{E}\left(-\frac{\partial}{\partial \beta_r}\frac{\partial}{\partial \beta_s}\ell(\beta,\phi)\right), \qquad r,s = 1,\dots,p.$$

- Thus, the Fisher information matrix substantially simplifies because $\mathbb{E}(Y_i) = \mu_i$, obtaining:

$$i_{rs} = \sum_{i=1}^n \frac{1}{a_i(\phi)}\frac{\partial \mu_i}{\partial \beta_s}\frac{\partial \theta_i}{\partial \beta_r}, \qquad r,s = 1,\dots,p.$$

Observed and expected information II 📖

- In the previous slides we already computed the explicit values of these derivatives:

$$\frac{\partial \mu_i}{\partial \beta_s} = \frac{x_{is}}{g'(\mu_i)}, \qquad \frac{\partial \theta_i}{\partial \beta_r} = \frac{x_{is}}{v(\mu_i)g'(\mu_i)}.$$

Combining the above equations, we obtain that the **Fisher information** $\boldsymbol{I}$ of a GLM has entries

$$i_{rs} = \frac{1}{\phi}\sum_{i=1}^n \omega_i \frac{x_{ir}x_{is}}{v(\mu_i)g'(\mu_i)^2} = \sum_{i=1}^n \frac{x_{ir}x_{is}}{\mathrm{var}(Y_i)g'(\mu_i)^2}, \qquad r, s = 1, \dots, p.$$

In **matrix notation**, we have that

$$\boldsymbol{I} = \boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X},$$

where $\boldsymbol{W} = \mathrm{diag}(w_1, \dots, w_n)$ and w_i are **weights** such that

$$w_i = \frac{1}{\phi}\frac{\omega_i}{v(\mu_i)g'(\mu_i)^2} = \frac{1}{\mathrm{var}(Y_i)g'(\mu_i)^2}, \qquad i = 1, \dots, n.$$

Canonical link: simplifications 📖

Under the **canonical link** we have that $\theta_i = x_{i1}\beta_1 + \cdots + \beta_p x_{ip}$, which means that

$$\frac{\partial^2 \theta_i}{\partial \beta_r \partial \beta_s} = 0 \qquad \Longrightarrow \qquad i_{rs} = j_{rs} = \sum_{i=1}^{n} \frac{1}{a_i(\phi)} \frac{\partial \mu_i}{\partial \beta_s} \frac{\partial \theta_i}{\partial \beta_r}.$$

The **observed information** $\boldsymbol{J}$ is **non-stochastic**, which means that observed information and expected (Fisher) information coincide, that is $i_{rs} = j_{rs}$ and $\boldsymbol{I} = \boldsymbol{J}$.

Under the **canonical link**, we also have the simplifications $1/v(\mu_i) = g'(\mu_i)$, yielding

$$i_{rs} = \frac{1}{\phi} \sum_{i=1}^{n} \omega_i v(\mu_i) x_{ir} x_{is}, \qquad r, s = 1, \dots, p.$$

In **matrix notation**, we have that $\boldsymbol{I} = \boldsymbol{X}^T \boldsymbol{W} \boldsymbol{X}$ with weights

$$w_i = \frac{1}{\phi} \omega_i v(\mu_i) = \frac{v(\mu_i)}{a_i(\phi)}, \qquad i = 1, \dots, n.$$

Further considerations

- The **observed** and **expected** information matrices $\boldsymbol{J}$ and $\boldsymbol{I}$, as well as weights $\boldsymbol{W}$, **depend** on β and ϕ. We write $\hat{\boldsymbol{J}}$, $\hat{\boldsymbol{I}}$ and $\hat{\boldsymbol{W}}$ to indicate that β and ϕ have been estimated with $\hat{\beta}$ and $\hat{\phi}$.

- If $\boldsymbol{X}$ has **full rank** and $g'(\mu) \neq 0$, then $\boldsymbol{I}$ is **positive definite** for any value of β and ϕ.

- Under the **canonical link**, we have $\boldsymbol{J} = \boldsymbol{I}$, and both matrices are **positive definite** if $\mathrm{rk}(\boldsymbol{X}) = p$.
- This implies that the log-likelihood function is **concave** because its second derivative is negative definite, so any **solution** to the **estimating equations** is also a **global optimum**.

- The Fisher information matrix could be computed exploiting **Bartlett identity**, namely

$$i_{rs} = \mathbb{E}\left[\left(\frac{\partial}{\partial \beta_r}\ell(\beta, \phi)\right)\left(\frac{\partial}{\partial \beta_s}\ell(\beta, \phi)\right)\right], \qquad r, s = 1, \dots, p.$$

as in Agresti (2015). Of course, the final result **coincide** with ours.

☠️ - Orthogonality of β and ψ

- Let us now consider the case in which ϕ is **unknown** so that $a_i(\phi) = \phi/\omega_i$. We obtain:

$$j_{r\phi} = -\frac{\partial}{\partial \beta_r}\frac{\partial}{\partial \phi}\ell(\beta, \phi) = \frac{1}{\phi^2}\sum_{i=1}^n \omega_i(y_i - \mu_i)\frac{\partial \theta_i}{\partial \beta_r}, \qquad r = 1, \dots, p.$$

  whose **expected value** is $i_{r\phi} = \mathbb{E}(j_{r\phi}) = 0$ since $\mathbb{E}(Y_i) = \mu_i$.

- This means the Fisher information matrix accounting for ϕ takes the form:

$$\begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & i_{\phi\phi} \end{pmatrix} \qquad \Longrightarrow \qquad \begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & i_{\phi\phi} \end{pmatrix}^{-1} = \begin{pmatrix} \boldsymbol{I}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & 1/i_{\phi\phi} \end{pmatrix}$$

  where $[\boldsymbol{I}]_{rs} = i_{rs}$ are the elements associated to β as before.

> The parameters β and ϕ are **orthogonal** and their estimates are **asymptotically independent**.
>
> Moreover, the matrices $\boldsymbol{I}$ and $\boldsymbol{I}^{-1}$ are sufficient for inference on β and there is no need to compute $i_{\phi\phi}$. Moreover, the maximum likelihood $\hat{\beta}$ can also be computed without knowing ϕ.

IRLS algorithm

Numerical methods for maximum likelihood estimation

- In general, the estimating equations of a GLM

  $$\boldsymbol{D}^T \boldsymbol{V}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}) = \mathbf{0}$$

  cannot be solved in **closed form** and we need to rely on **numerical methods**.
- An **iterative** method means that we start the **algorithm** with a candidate value $\beta^{(1)}$ (**initialization**). Then, at the step t we update

  $$\beta^{(t+1)} = \texttt{update}(\beta^{(t)}), \qquad t = 1, 2, \dots$$

- The algorithm **stops** whenever a certain criteria is met, e.g. when $||\beta^{(t+1)} - \beta^{(t)}|| < \epsilon$, where ϵ is sometimes called **tolerance**. We say it reached **convergence**.
- The **iteratively re-weighted least squares** (IRLS) algorithm became very popular after being proposed by Nelder and Wedderburn (1972) and is currently implemented in **R**.
- The IRLS algorithm can be used for any GLM, has a clear geometric interpretation, and often delivers good performance. It can be seen as a **variant** of **Newton-Raphson**.

Newton-Raphson algorithm I

- In the Newton-Raphson algorithm, we consider a second-order **Taylor expansion** of the log-likelihood $\ell(\beta) = \ell(\beta, \phi)$ centered in $\beta^{(t)}$, namely:

$$\ell(\beta) \approx \ell(\beta^{(t)}) + \ell_*(\beta^{(t)})^T(\beta - \beta^{(t)}) - \frac{1}{2}(\beta - \beta^{(t)})^T \boldsymbol{J}^{(t)}(\beta - \beta^{(t)})$$

  where $\ell_*(\beta^{(t)})$ is the **score function** and $\boldsymbol{J}^{(t)}$ is the **observed information**, evaluated at $\beta^{(t)}$.

- In other words, we **approximate** the log-likelihood $\ell(\beta)$ with a **parabola**. This gives the **approximate likelihood equations**:

$$\ell_*(\beta^{(t)}) - \boldsymbol{J}^{(t)}(\beta - \beta^{(t)}) = \mathbf{0}.$$

- Solving the equation above gives the following **updates**:

$$\beta^{(t+1)} = \hat{\beta}^{(t)} + (\boldsymbol{J}^{(t)})^{-1}\ell_*(\beta^{(t)}), \qquad t = 1, 2, \dots$$

> The Netwon-Raphson method essentially considers a series of **parabolic approximations** to the log-likelihood, each time evaluating the **point of maximum**.

Newton-Raphson algorithm II

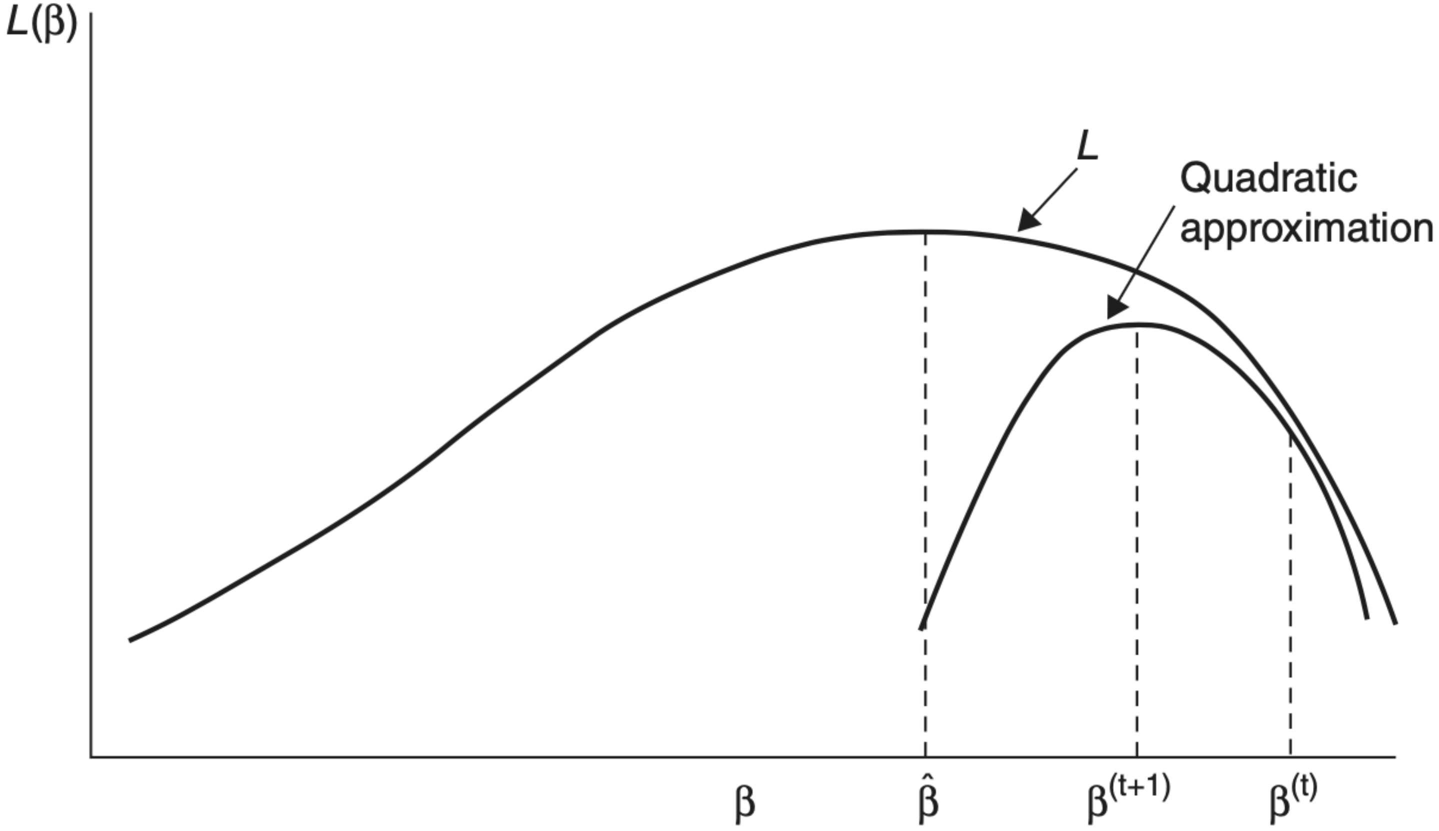


Figure 4.2 Illustration of a cycle of the Newton–Raphson method.

- Figure taken from Agresti (2015).

Iteratively re-weighted least squares I 📖

- The matrix $\boldsymbol{J}^{(t)}$ is not always invertible, therefore the algorithm may crash. To remedy this, we replace it with the **expected information** $\boldsymbol{I}^{(t)}$.

> In the **iteratively re-weighted least squares** (IRLS) algorithm, we consider the updates:
>
> $$\beta^{(t+1)} = \beta^{(t)} + (\boldsymbol{I}^{(t)})^{-1}\ell_*(\beta^{(t)}), \qquad t = 1, 2, \dots$$
>
> This method is also called **Fisher scoring**.

- The above formula can **simplified** a bit. First, we rewrite the **score** as

$$\frac{\partial}{\partial \beta_r}\ell(\beta, \phi) = \frac{1}{\phi}\sum_{i=1}^n \omega_i \frac{(y_i - \mu_i)}{v(\mu_i)}\frac{x_{ir}}{g'(\mu_i)} = \sum_{i=1}^n x_{ir} w_i (y_i - \mu_i) g'(\mu_i),$$

where the **weights** were defined as $w_i = \omega_i/(\phi v(\mu_i) g'(\mu_i)^2)$. In **matrix notation** we will write:

$$\ell_*(\beta^{(t)}) = \boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{u}^{(t)}, \qquad \boldsymbol{I}^{(t)} = \boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{X},$$

where $\boldsymbol{u}^{(t)} = (u_1^t, \dots, u_n^{(t)})^T$ and $u_i^{(t)} = (y_i - \mu_i^{(t)}) g'(\mu_i^{(t)})$ for $i = 1, \dots, n$.

Iteratively re-weighted least squares II 📖

- Exploiting the former formulas, we can write the IRLS update as follows
$$\beta^{(t+1)} = \beta^{(t)} + (\boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{u}^{(t)}.$$
Now **multiply** both sides by $(\boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{X})$, **simplify** and **re-arrange** the resulting terms. This gives the following formula.

In the **iteratively re-weighted least squares** (IRLS) algorithm, we consider the updates:

$$\beta^{(t+1)} = (\boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{z}^{(t)}, \qquad t = 1, 2, \dots,$$

where $\boldsymbol{z}^{(t)} = (z_1^{(t)}, \dots, z_n^{(t)})$ is called **pseudo-response** whose elements are defined as

$$z_i^{(t)} = \boldsymbol{x}_i^T\hat{\beta}^{(t)} + u_i^{(t)} = \boldsymbol{x}_i^T\hat{\beta}^{(t)} + (y_i - \mu_i^{(t)})g'(\mu_i^{(t)}), \qquad i = 1, \dots, n.$$

Hence, each update can be interpreted as the solution of a **weighted least square** problem:

$$\beta^{(t+1)} = \arg\min_{\beta \in \mathbb{R}^p} (\boldsymbol{z}^{(t)} - \boldsymbol{X}\beta)^T\boldsymbol{W}^{(t)}(\boldsymbol{z}^{(t)} - \boldsymbol{X}\beta).$$

Iteratively re-weighted least squares III 📖

- The IRLS updates does not depend on the choice of ϕ, because it **cancels** in the multiplications, as we would expect.

- The pseudo-responses have a **nice interpretation**, because they can be interpreted as a linear approximation of the transformed responses:

$$g(y_i) \approx g(\mu_i) + (y_i - \mu_i)g'(\mu_i) = \eta_i + (y_i - \mu_i)g'(\mu_i) = z_i.$$

- Based on this approximation, a good **initialization** is

$$\boldsymbol{W}^{(1)} = I_n, \qquad z_i^{(1)} = g(y_i), \qquad \Longrightarrow \qquad \beta^{(2)} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T g(\boldsymbol{y}),$$

  the **least square** solution for the transformed data. To avoid boundary issues, sometimes the data are perturbed, as we did in Binomial regression.

Example: IRLS for logistic regression

- Consider a **logistic regression** model for **proportions** $Y_i \in \{0, 1/m_i, \dots, 1\}$ with probability of success $\pi_i = \mu_i$ and trials m_i.

IRLS algorithm for logistic regression

- **Initialize** $\boldsymbol{\beta}^{(1)} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T \text{logit}(\tilde{\boldsymbol{y}})$ where $\text{logit}(\tilde{\boldsymbol{y}})$ is the **empirical logit** transform.
- For $t = 1, 2, \dots$ until **convergence** compute:

$$\beta^{(t+1)} = (\boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{W}^{(t)}\boldsymbol{z}^{(t)},$$

where the weights in $\boldsymbol{W}^{(t)}$ equals $w_i^{(t)} = m_i\pi_i^{(t)}(1 - \pi_i^{(t)})$ and the **pseudo-responses** $\boldsymbol{z}^{(t)}$ are

$$z_i^{(t)} = \boldsymbol{x}_i^T\beta^{(t)} + \frac{y_i - \pi_i^{(t)}}{\pi_i^{(t)}(1 - \pi_i^{(t)})}, \qquad i = 1, \dots, n,$$

with probabilities $\pi_i^{(t)} = \exp(\boldsymbol{x}_i^T\beta^{(t)})/(1 + \exp(\boldsymbol{x}_i^T\beta^{(t)}))$ for $i = 1, \dots, n$.

Estimation of the dispersion ϕ

- In some GLMs, such as the Gaussian and the Gamma, there is a **dispersion parameter** ϕ that we need to estimate.
- Instead of the maximum likelihood, because of **numerical instabilities** and **lack of robustness** it is typically preferred a **method of moments** estimator. If μ_i were known, the estimator

$$\frac{1}{n}\sum_{i=1}^n \omega_i \frac{(y_i - \mu_i)^2}{v(\mu_i)}$$

would be **unbiased** for ϕ, because $\mathbb{E}\{(Y_i - \mu_i)^2\} = (\phi/\omega_i)v(\mu_i)$. This motivates the estimator

$$\hat{\phi} = \frac{1}{n-p}\sum_{i=1}^n \omega_i \frac{(y_i - \hat{\mu}_i)^2}{v(\hat{\mu}_i)}, \qquad \hat{\mu}_i = g^{-1}(\boldsymbol{x}_i^T\hat{\beta}).$$

- This is a **consistent** estimator of ϕ as long as $\hat{\beta}$ is consistent.
- When $g(\mu_i) = \mu_i$ is the **identity link** and $v(\mu_i) = \omega_i = 1$, this coincides with the usual unbiased estimator s^2 of σ^2 for a Gaussian linear model.

Inference and hypothesis testing

Asymptotic distribution of $\hat{\beta}$

> The **asymptotic distribution** of the **maximum likelihood estimator** is
>
> $$\hat{\beta} \dot{\sim} \mathrm{N}_p\left(\beta, (\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}\right),$$
>
> for large values of n and under mild regularity conditions on $\boldsymbol{X}$.

- Under correct specification and mild conditions on $\boldsymbol{X}$, the maximum likelihood estimator is **asymptotically unbiased** and with known asymptotic **variance**

$$\mathbb{E}(\hat{\beta} - \beta) \approx 0, \qquad \mathrm{var}(\hat{\beta}) \approx (\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}.$$

- In practice, since $\boldsymbol{W}$ depends on β and ϕ, we rely on the following approximation

$$\widehat{\mathrm{var}}(\hat{\beta}) = (\boldsymbol{X}^T\hat{\boldsymbol{W}}\boldsymbol{X})^{-1},$$

where we plugged in the estimates $\hat{\beta}$ and $\hat{\phi}$ into $\boldsymbol{W}$ obtaining $\hat{\boldsymbol{W}}$. The **standard errors** are:

$$\texttt{Std. Error} = [\widehat{\mathrm{se}}(\hat{\beta})]_j = \sqrt{[(\boldsymbol{X}^T\hat{\boldsymbol{W}}\boldsymbol{X})^{-1}]_{jj}}$$

Example: Beetles data

- Using the Beetles data, we specified a **binomial logistic** regression model for the counts $m_i Y_i \sim \text{Binomial}(m_i, \pi_i)$ with mean $\mu_i = \exp(\beta_1 + \beta_2 x_i)/(1 + \exp(\beta_1 + \beta_2 x_i))$.
- We previously **estimated** $\hat{\beta} = (-60.717, 34.270)$. This means that the **weights** are estimated as

$$\hat{\boldsymbol{W}} = \text{diag}(m_1 \hat{\mu}_1(1 - \hat{\mu}_1), \dots, m_n \hat{\mu}_n(1 - \hat{\mu}_n)) = \text{diag}(3.255, 8.227, \dots, 1.231).$$

  from which we obtain the **estimated Fisher information matrix**:

$$\boldsymbol{X}^T \hat{\boldsymbol{W}} \boldsymbol{X} = \begin{pmatrix} \sum_{i=1}^n m_i \hat{\mu}_i(1 - \hat{\mu}_i) & \sum_{i=1}^n x_i m_i \hat{\mu}_i(1 - \hat{\mu}_i) \\ \sum_{i=1}^n x_i m_i \hat{\mu}_i(1 - \hat{\mu}_i) & \sum_{i=1}^n x_i^2 m_i \hat{\mu}_i(1 - \hat{\mu}_i) \end{pmatrix} = \begin{pmatrix} 58.484 & 104.011 \\ 104.011 & 185.095 \end{pmatrix}.$$

- Hence, the **estimated covariance** matrix of the maximum likelihood estimator is

$$\widehat{\text{var}}(\hat{\beta}) = (\boldsymbol{X}^T \hat{\boldsymbol{W}} \boldsymbol{X})^{-1} = \begin{pmatrix} 26.840 & -15.082 \\ -15.082 & 8.481 \end{pmatrix}.$$

- Therefore the **estimated standard errors** are

$$[\widehat{\text{se}}(\hat{\beta})]_j = \sqrt{[(\boldsymbol{X}^T \hat{\boldsymbol{W}} \boldsymbol{X})^{-1}]_{jj}} \quad \Longrightarrow \quad \widehat{\text{se}}(\hat{\beta}) = (5.181, 2.912).$$

Example: Aids data

- In the Aids data, we specified a **Poisson** regression model with $\mathbb{E}(Y_i) = \exp(\beta_1 + \beta_2 x_i)$ and estimated $\hat{\beta} = (0.304, 0.259)$.
- This means that the weights are estimated as

$$\hat{\boldsymbol{W}} = \text{diag}(\hat{\mu}_1, \dots, \hat{\mu}_n) = \text{diag}(1.755, \dots, 50.863).$$

from which we obtain the **estimated Fisher information matrix**:

$$\boldsymbol{X}^T \hat{\boldsymbol{W}} \boldsymbol{X} = \begin{pmatrix} \sum_{i=1}^n \hat{\mu}_i & \sum_{i=1}^n x_i \hat{\mu}_i \\ \sum_{i=1}^n x_i \hat{\mu}_i & \sum_{i=1}^n x_i^2 \hat{\mu}_i \end{pmatrix} = \begin{pmatrix} 217 & 2387 \\ 2387 & 28279.05 \end{pmatrix}.$$

- Hence, the **estimated covariance** matrix of the maximum likelihood estimator is

$$\widehat{\text{var}}(\hat{\beta}) = (\boldsymbol{X}^T \hat{\boldsymbol{W}} \boldsymbol{X})^{-1} = \begin{pmatrix} 0.06445 & -0.00544 \\ -0.00544 & 0.00049 \end{pmatrix}.$$

- Therefore the **estimated standard errors** are

$$[\widehat{\text{se}}(\hat{\beta})]_j = \sqrt{[(\boldsymbol{X}^T \hat{\boldsymbol{W}} \boldsymbol{X})^{-1}]_{jj}} \quad \Longrightarrow \quad \widehat{\text{se}}(\hat{\beta}) = (0.254, 0.022).$$

Wald test and confidence intervals

- Consider the **hypothesis** $H_0 : \beta_j = \beta_0$ against the **alternative** $H_1 : \beta_j \neq \beta_0$. The **Wald test statistic** z_j, rejecting the hypothesis for large values of $|z_j|$ is:

$$\texttt{z value} = z_j = \frac{\hat\beta_j - \beta_0}{[\widehat{\mathrm{se}}(\hat\beta)]_j} = \frac{\hat\beta_j - \beta_0}{\sqrt{[(\boldsymbol{X}^T\hat{\boldsymbol{W}}\boldsymbol{X})^{-1}]_{jj}}} \,\dot\sim\, \mathrm{N}(0,1).$$

  which is **approximately** distributed as a **standard normal** under H_0.

- The **p-value** is defined in the usual way, namely

$$\alpha_{\text{obs}} = \mathbb{P}(Z \geq |z_j|) = 2(1 - \Phi(|z_j|)), \qquad Z \sim \mathrm{N}(0,1).$$

- By inverting the the Wald test, we obtain the associated **confidence interval**

$$\hat\beta_j \pm z_{1-\alpha/2}\sqrt{[(\boldsymbol{X}^T\hat{\boldsymbol{W}}\boldsymbol{X})^{-1}]_{jj}}.$$

  of **approximate** level $1-\alpha$, where $z_{1-\alpha/2}$ is the quantile of a standard Gaussian.

Comparison with the Gaussian linear model

- In a classical **Gaussian linear model** the weight matrix is $\boldsymbol{W} = \sigma^2 I_n$, therefore

$$\hat{\beta} \sim \mathrm{N}_p\left(\beta, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}\right).$$

- The **Wald statistic** z_j **specializes** to

$$z_j = \frac{\hat{\beta}_j - \beta_0}{[\widehat{\mathrm{se}}(\hat{\beta})]_j} = \frac{\hat{\beta}_j - \beta_0}{s\sqrt{[(\boldsymbol{X}^T\boldsymbol{X})^{-1}]_{jj}}},$$

which is the usual test statistic considered, e.g., in the output of `lm` in **R**.

- However, in the Gaussian case there is **no need** of **approximations**. The distribution of z_j is a **Student**' t_{n-p} under H_0, which indeed converges to a $\mathrm{N}(0,1)$ for large values of n.

> In GLMs we use procedures that are **approximate** rather than **exact**. Of course, whenever an exact result is known, we should use it.

Example: Beetles data

- The Wald test is the **default** choice in **R** for checking the hypotheses $H_0 : \beta_j = 0$. In the Beetles data we get the following familiar summary:

```
z test of coefficients:

            Estimate Std. Error z value  Pr(>|z|)    
(Intercept) -60.7175     5.1807 -11.720 < 2.2e-16 ***
logdose      34.2703     2.9121  11.768 < 2.2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

- Many of the above quantities (estimates and standard errors) have been obtained before.
- In this case, we **reject** the null hypothesis that $\beta_2 = 0$. Indeed, even from the scatterplot there was evidence of a relationship between the deaths proportion and the logdose.

- For completeness, we also compute the associated **Wald confidence intervals**, which are:

```
                2.5 %    97.5 %
(Intercept) -70.87144 -50.56347
logdose      28.56265  39.97800
```

Example: Aids data

- The Wald tests for checking the hypotheses $H_0 : \beta_j = 0$ in the Aids data are provided below.

```
z test of coefficients:

            Estimate Std. Error z value Pr(>|z|)    
(Intercept) 0.303655   0.253867  1.1961   0.2317    
period      0.258963   0.022238 11.6448   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

- In this case, we **reject** the null hypothesis that $\beta_2 = 0$ because the **p-value** `Pr(>|z|)` ≈ 0. Again, this is not very surprising: the number of deaths was clearly increasing over time.

- The associated **Wald confidence intervals** are:

```
                 2.5 %    97.5 %
(Intercept) -0.1939158 0.8012249
period       0.2153764 0.3025494
```

General hypothesis testing

- Suppose we wish to test **multiple parameters** at the same time. Let us organize the parameters into **two blocks**:

$$\beta = \begin{pmatrix} \beta_A \\ \beta_B \end{pmatrix}, \qquad \beta_A = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_{p_0} \end{pmatrix}, \quad \beta_B = \begin{pmatrix} \beta_{p_0+1} \\ \vdots \\ \beta_p \end{pmatrix},$$

where $q = p - p_0$ is the number of **constrained parameters**. We want to **test the hypothesis**:

$$H_0 : \beta_B = \beta_0 \qquad \text{against} \qquad H_1 : \beta_B \neq \beta_0.$$

A common case is $H_0 : \beta_B = 0$ (**nested models**), where we compare the **reduced model** M_0 against the **full model** M_1. We verify if **all** the q variables associated with β_B can be omitted.

The case $q = 1$, that is $\beta_B = \beta_p$ with $H_0 : \beta_p = 0$ corresponds to the previously considered situation where we test if a **specific coefficient**, say β_p, is non-zero.

Testing hypothesis in GLMs I

- There are **three classical tests** that we could consider for such a testing problem: the **Wald test** W_e , the **Rao-score test** W_u, and the **log-likelihood ratio test** W.
- All these tests **reject** the null hypothesis for **large values** of the **statistic**.

Wald test (general case)

Let $\hat{\beta} = (\hat{\beta}_A, \hat{\beta}_B)$ be the **unrestricted** maximum likelihood, the quantity

$$W_e = (\hat{\beta}_B - \beta_0)^T \, \widehat{\mathtt{var}}(\hat{\beta}_B)^{-1} \, (\hat{\beta}_B - \beta_0),$$

is called **Wald test**. Here $\widehat{\mathtt{var}}(\hat{\beta}_B)$ is the appropriate **block** of $(\boldsymbol{X}^T\hat{\boldsymbol{W}}\boldsymbol{X})^{-1}$ and $\hat{\boldsymbol{W}}$ is estimated using $\hat{\beta}$ and $\hat{\phi}$. Under H_0 this quantity is **approximately** distributed as

$$W_e \dot{\sim} \chi^2_q,$$

a χ^2 distribution with q **degrees of freedom**. The **p-value** is $\mathtt{Pr(>Chi)} = \mathbb{P}(W_e > w_{\text{e, obs}})$.

- Clearly, in the $q = 1$ case we recover the Wald statistic with $z_j^2 = W_e$.

Log-likelihood ratio test

Log-likelihood ratio test (LRT)

Let $\hat{\beta} = (\hat{\beta}_A, \hat{\beta}_B)$ be the **unrestricted** maximum likelihood and let $\hat{\beta}_0 = (\hat{\beta}_{A,0}, \beta_0)$ the **restricted** maximum likelihood estimate. The quantity

$$W = 2[\ell(\hat{\beta}; \hat{\phi}) - \ell(\hat{\beta}_0; \hat{\phi})],$$

is called **log-likelihood ratio** test (LRT). Under H_0 this quantity is **approximately** distributed as

$$W \dot{\sim} \chi^2_q,$$

a χ^2 distribution with q **degrees of freedom**. The **p-value** is `Pr(>Chi)` $= \mathbb{P}(W > w_{\text{obs}})$.

- When testing $H_0 : \beta_B = 0$, we separately fit the **full model**, obtaining $\hat{\beta}$, and the **reduced model**, obtaining $\hat{\beta}_0 = (\hat{\beta}_{A,0}, 0)$. Then, we compare their log-likelihoods: $\ell(\hat{\beta}; \hat{\phi}) - \ell(\hat{\beta}_0; \hat{\phi})$.
- The LRT is the **default** in **R** for comparing **nested models**.

When the dispersion parameter ϕ is unknown, a **variant** uses **separate estimates** $\hat{\phi}$, based on $\hat{\beta}$, and $\hat{\phi}_0$, based on $\hat{\beta}_0$. The `anova` **R** command uses a single $\hat{\phi}$, as described above.

Score or Rao test

Rao-score test

Let $\hat\beta = (\hat\beta_A, \hat\beta_B)$ be the **unrestricted** maximum likelihood and let $\hat\beta_0 = (\hat\beta_{A,0}, \beta_0)$ the **restricted** maximum likelihood estimate. Moreover, let

$$\ell_B(\beta;\phi) = \frac{\partial}{\partial \beta_B}\ell(\beta,\phi),$$

namely the block of the score function associated with β_B. The quantity

$$W_u = \ell_B(\hat\beta_0;\hat\phi)^T\, \widetilde{\mathrm{var}}(\hat\beta_B)\, \ell_B(\hat\beta_0;\hat\phi),$$

is called **Rao-score test**. Here $\widetilde{\mathrm{var}}(\hat\beta_B)$ is the appropriate block of $(\boldsymbol{X}^T\tilde{\boldsymbol{W}}\boldsymbol{X})^{-1}$ where $\tilde{\boldsymbol{W}}$ is estimated using the **restricted** $\hat\beta_0$. Under H_0 this quantity is **approximately** distributed as

$$W_u \,\dot\sim\, \chi^2_q,$$

a χ^2 distribution with q **degrees of freedom**. The **p-value** is `Pr(>Chi)` $= \mathbb{P}(W_u > w_{\text{u, obs}})$.

The Rao-score test arguably the **less common**. When ϕ is unknown, there are several variants depending on how it is estimated.

A graphical representation when $p = 1$

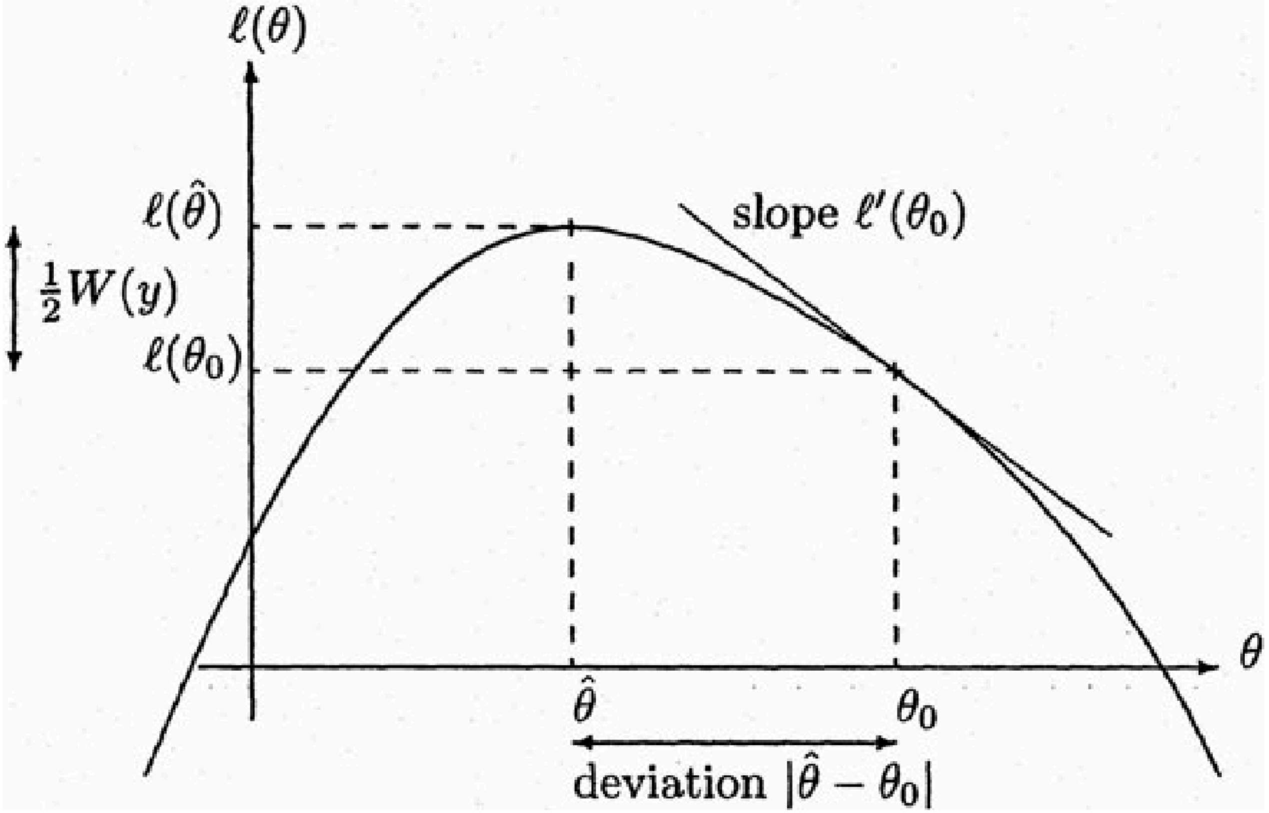


Figure 4.2 *Three test functions connected to the log-likelihood*

- Figure taken from Azzalini (1996). This is also the cover of the **book**!

Three asymptotically equivalent tests

The Wald test, the Score test and the log-likelihood ratio test are **asymptotically equivalent**, that is, these tests give the **same number** for large values of n. We have that

$$W_e = W + o_p(1), \qquad W_u = W + o_p(1),$$

where $o_p(1)$ is a quantity that goes to 0 in probability as $n \to \infty$.

- When $q = 1$, we can also **invert** W_e, W_u and W tests over β_0 to obtain the corresponding **confidence interval**. This is often done **numerically** for W_u and W.
- The Wald test depends on the parametrization. When considering a transformation of β, the variance must be adjusted using the derivative of the transformation (**delta method**).[1]
- On the other hand, both the LRT and the score are **invariant**, and therefore we can simply **transform** the **extremes** of the **original interval** without further corrections.

[1] Transforming the extremes of Wald confidence interval "works" in the sense that it produces a valid confidence interval, but it is **not** the Wald interval in the trasformed scale.

Comparison with the Gaussian linear model

In the Gaussian linear model all tests are **equivalent** if $\phi = \sigma^2$ is **known**. We have

$$W = W_e = W_u = \frac{||\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}_0||^2 - ||\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}||^2}{\sigma^2} \sim \chi^2_q.$$

The χ^2_q distribution is **exact** and not an approximation thanks to Cochran theorem.

- Consider the **log-likelihood ratio** for testing $H_0 : \beta_B = \beta_0$. Suppose σ^2 is **unknown**, then:

  $$W = 2[\ell(\hat{\beta}; \hat{\phi}) - \ell(\hat{\beta}_0; \hat{\phi})] = \frac{||\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}_0||^2 - ||\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}||^2}{\hat{\phi}} = q\frac{(||\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}_0||^2 - ||\boldsymbol{y} - \boldsymbol{Y}\hat{\beta}||^2)/q}{||\boldsymbol{y} - \boldsymbol{X}\hat{\beta}||^2/(n-p)}$$
  $$= qF,$$

  where $F \sim F_{q,n-p}$ is the usual **Snedecor**'s F. Indeed qF is **approximately** distributed as χ^2_q for large values of n.

- The quantities W_e, W_u, and W are the natural extension of the F-statistic for GLMs. They are **approximately** distributed as χ^2_q with q **degrees of freedom**.

Example: Beetles data

- We would like to use the **Wald**, the **Rao-score** and the **log-likelihood ratio** tests to verify the hypothesis $H_0 : \beta_2 = 0$, that is the relevance of `logdose` in predicting the response.

- In this case, we have $q = 1$ (`Df`) because there is only one parameter under scrutiny.

Test for the hypothesis $H_0 : \beta_2 = 0$	`Chi`	`Df`	`Pr(>Chi)`
W_e - **Wald test**	138.488	1	≈ 0
W_u - **Rao-score test**	227.580	1	≈ 0
W - **Log-likelihood ratio test**	272.970	1	≈ 0

- As one may expect, the test values are not identical. Here the sample size is $n = 8$, which is definitely not a big number, therefore we are far from the **asymptotic regime**.
- However, the practical conclusions are identical. All tests strongly **reject** the null hypothesis.

- We previously obtained the **Wald statistic** z_j and indeed $z_j^2 = 11.76811^2 = 138.488 = W_e$.

Example: Beetles data

- Any statistical test can be **inverted**, namely we find all the values β_0 such that we do **not reject the null hypothesis**. This generates a **confidence interval**.

- For the Wald test, the inversion is done analytically, producing the "usual" confidence interval.
- For the Rao-score and the log-likelihood ratio we need numerical procedures.
- In the `Beetles` data, the three tests produce the following confidence intervals for β_2, associated to `logdose`.

Confidence intervals for β_2 at a 95% level	**2.5%**	**97.5%**
W_e - **Wald test**	28.563	39.978
W_u - **Rao-score test**	28.588	39.957
W - **Log-likelihood ratio test**	28.854	40.301

- Wald interval was also computed before. The three tests produce **nearly identical** intervals.
- Wald is always symmetric around $\hat{\beta}_j$, whereas Rao and the log-likelihood ratio are typically **asymmetric**, depending on the shape of the likelihood function.

Example: Aids data

- Let us know perform the same analysis for the Aids data. Again, we test the null hypothesis $H_0 : \beta_2 = 0$, which is the relevance of period in predicting the response.

Test for the hypothesis $H_0 : \beta_2 = 0$	Chi	Df	Pr(>Chi)
W_e - Wald test	135.602	1	≈ 0
W_u - Rao-score test	163.586	1	≈ 0
W - Log-likelihood ratio test	178.551	1	≈ 0

- As before, despite their numerical differences, all the tests **reject** the null hypothesis. We previously obtained the **Wald statistic** $z_j = 11.645$ and indeed $z_j^2 = 11.645^2 = 135.6 = W_e$.

Confidence intervals for β_2 at a 95% level	2.5%	97.5%
W_e - Wald test	0.2154	0.3025
W_u - Rao-score test	0.2155	0.3025
W - Log-likelihood ratio test	0.2165	0.3037

Example: Aids data

- We are actually interested in a confidence interval for the quantity $100 \times (\exp(\beta_2) - 1)$, which is the **percentage increase** of deaths after each period.
- Thanks to **invariance property** of the Rao-score and the log-likelihood ratio tests, we can simply **transform** the **original intervals** for β_2.
- If the extremes of the log-likelihood ratio interval are $C_{\text{low}}, C_{\text{high}}$, then the new interval is

$$[100 \times (\exp(C_{\text{low}}) - 1),\ 100 \times (\exp(C_{\text{high}}) - 1)].$$

and similarly for the Rao-score case. These are reported below.

Confidence intervals for $100[\exp(\beta_2) - 1]$ at a 95% level	**2.5%**	**97.5%**
W_u - **Rao-score test**	24.04	35.32
W - **Log-likelihood ratio test**	24.17	35.49

- The **average** percentage increase is between 24% and 35% each period, with a 95% **confidence**.
- These confidence intervals are always **positive**, which is desirable because they are percentages.

Example: Aids data

- In the Wald case, we cannot simply transform the extremes of the intervals. Indeed, that would lead to a **valid** confidence interval that is not anymore of Wald type (*Lo sbagliato* 🥃).
- Instead, we first need to **adjust** the **variance** according to the **delta method**, obtaining

$$\widehat{\text{var}}\{100[\exp(\hat{\beta}_2)-1]\} = 100^2 \exp(2\hat{\beta}_2)\text{var}(\hat{\beta}_2) = 8.301184.$$

- The Wald confidence interval for $100[\exp(\hat{\beta}_2)-1]$ therefore is

$$100[\exp(\hat{\beta}_2)-1] \pm z_{1-\alpha/2}\widehat{\text{se}}\{100[\exp(\hat{\beta}_2)-1]\}.$$

Confidence intervals for $100[\exp(\beta_2)-1]$ **at a** 95% **level**	**2.5%**	**97.5%**
W_e - **Wald test**	23.91	35.21
"*Lo sbagliato*" - transformed Wald	24.03	35.33

> Whenever there are restrictions on the parametric space, as in this case, Wald is typically **problematic**. Here, it **could** lead to **negative values**, which is absurd.

Deviance, model checking, residuals

Deviance: some intuitions

- In a Gaussian linear model, we called **deviance** the residual sum of squares, that is

$$D(\boldsymbol{y};\hat{\boldsymbol{\mu}}) = \sum_{i=1}^n (y_i - \boldsymbol{x}_i^T\hat{\beta})^2 = \sum_{i=1}^n (y_i - \hat{\mu}_i)^2.$$

- The residual sum of squares $D(\boldsymbol{y};\hat{\boldsymbol{\mu}})$ is a **goodness of fit** measure. The lower the deviance, the higher the quality of the predictions.

- When σ^2 is **known**, the distribution of the **scaled deviance** is

$$\frac{D(\boldsymbol{Y};\hat{\boldsymbol{\mu}})}{\sigma^2} = \frac{1}{\sigma^2}\sum_{i=1}^n (Y_i - \boldsymbol{x}_i^T\hat{\beta})^2 \sim \chi^2_{n-p}.$$

- When σ^2 is known, the difference of scaled deviances of two nested models is:

$$W = \frac{D(\boldsymbol{Y};\hat{\boldsymbol{\mu}}_0) - D(\boldsymbol{Y};\hat{\boldsymbol{\mu}})}{\sigma^2} = \frac{||\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}_0||^2 - ||\boldsymbol{Y} - \boldsymbol{X}\hat{\beta}||^2}{\sigma^2} \sim \chi^2_q.$$

- The natural question is: what is a natural **generalization** of the deviance for GLMs?

Example: Beetles data, saturated model

- Let us consider again the Beetles data and the predictions $\hat{\mu}_i$, based on $p = 2$ parameters. These predictions are not perfect but that may be due to chance.

m_i	deaths (S_i)	logdose (x_i)	$Y_i = S_i/m_i$	$\hat{\mu}_i$
59	6	1.691	0.102	0.059
60	13	1.724	0.217	0.164
62	18	1.755	0.290	0.362
56	28	1.784	0.500	0.605
63	52	1.811	0.825	0.795
59	53	1.837	0.898	0.903
62	61	1.861	0.984	0.955
60	60	1.884	1.000	0.979

- The **empirical proportions** s_i/m_i can be seen as **estimates** of the **most flexible model**, in which every observation Y_i has its own mean μ_i. We call it **saturated model** because $p = n$.

Saturated model

- Let us express the **log-likelihood** of a GLM as a function of the mean $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)$.
- When evaluated in the maximum likelihood, this gives:

$$\ell_{\mathcal{M}}(\hat{\boldsymbol{\mu}}, \phi) = \sum_{i=1}^{n} \omega_i \frac{y_i \theta(\hat{\mu}_i) - b(\theta(\hat{\mu}_i))}{\phi} + c(y_i, \phi).$$

  The maximum likelihood for each μ_i is **restricted**, in the sense that depends on the p parameters of the **linear predictor** $\boldsymbol{x}_i^T \beta$ through the link function $g(\mu_i) = \boldsymbol{x}_i^T \beta$.

- In the **saturated model** the means μ_i are **unrestricted**: each parameter is estimated separately, giving the maximum likelihood estimate $\hat{\mu}_{i,\text{sat}} = y_i$. This happens whenever $p = n$.
- When evaluated in the maximum, the log-likelihood of the saturated model is

$$\ell_{\mathcal{M}}(\boldsymbol{y}, \phi) = \sum_{i=1}^{n} \omega_i \frac{y_i \theta(y_i) - b(\theta(y_i))}{\phi} + c(y_i, \phi).$$

- The saturated model is the **most complex model** we can think of.

Deviance

The **deviance** of a GLM is defined as

$$\begin{aligned} D(\boldsymbol{y};\hat{\boldsymbol{\mu}}) := \phi W &= \phi\, 2[\ell_{\mathcal{M}}(\boldsymbol{y},\phi) - \ell_{\mathcal{M}}(\hat{\boldsymbol{\mu}},\phi)] \\ &= 2\sum_{i=1}^{n}\omega_i \left\{y_i[\theta(y_i) - \theta(\hat{\mu}_i)] - [b(\theta(y_i)) - b(\theta(\hat{\mu}_i))]\right\}. \end{aligned}$$

The quantity $D(\boldsymbol{y};\hat{\boldsymbol{\mu}})/\phi$ is called **scaled deviance** and it corresponds to a **log-likelihood ratio test** W in which the current model is tested against the saturated model.

- By definition, the deviance is **positive**: $D(\boldsymbol{y};\hat{\boldsymbol{\mu}}) \geq 0$, because $\ell_{\mathcal{M}}(\boldsymbol{y},\phi) \geq \ell_{\mathcal{M}}(\hat{\boldsymbol{\mu}},\phi)$.
- The deviance of the saturated model is $D(\boldsymbol{y};\boldsymbol{y}) = 0$.

- The deviance describes a **lack of fit**: the higher the deviance, the poorer the fit.
- It measures the discrepancy between the saturated model and a model using $p < n$ parameters.

- The deviance is a function of $\boldsymbol{\mu}$, therefore its definition does not depend on the link function $g(\cdot)$.

Deviance and log-likelihood ratio test

Let us consider two **nested models** $M_0 \subset M_1$. The **reduced model** M_0 has p_0 parameters and predictions $\hat{\boldsymbol{\mu}}_0$. The **full model** M_1 has p parameters $\hat{\boldsymbol{\mu}}_1$.

The **log-likelihood ratio test** W for testing model M_0 against model M_1[1] can be written as

$$W = 2[\ell_{\mathcal{M}}(\hat{\boldsymbol{\mu}}, \hat{\phi}) - \ell_{\mathcal{M}}(\hat{\boldsymbol{\mu}}_0, \hat{\phi})] = \frac{D(\boldsymbol{Y}; \hat{\boldsymbol{\mu}}_0) - D(\boldsymbol{Y}; \hat{\boldsymbol{\mu}})}{\hat{\phi}} \,\dot{\sim}\, \chi^2_q.$$

where $q = p - p_0$ are the degrees of freedom.

- The log-likelihood ratio can be interpreted as a difference of scaled deviances. This explains why it is popular in GLMs for comparing nested models.
- This is also strong parallelism with the Gaussian linear model.

[1] More formally, we should say that we are testing the hypothesis $H_0 : \beta_B = \mathbf{0}$ against the alternative $H_1 : \beta_B \neq \mathbf{0}$. I hope you can tolerate this slight linguistic abuse.

The null model

Let us consider a model M_{null} with **no covariates** and one parameter $(p = 1)$, i.e. the **intercept**. The predicted values are all equals to

$$\hat{\boldsymbol{\mu}}_{\text{null}} = (g^{-1}(\hat{\beta}_1), \dots, g^{-1}(\hat{\beta}_1)).$$

We call M_{null} the **null model** and $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}_{\text{null}})$ the **null deviance**.

- The null model is the “opposite” of the saturated model. It is the **simplest** among all models and the one having the **highest deviance**.
- Indeed, the following inequalities hold:

$$0 = D(\boldsymbol{y}; \boldsymbol{y}) \leq D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) \leq D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}_{\text{null}}).$$

- It is sometimes useful to test the current model against the null model:

$$W = \frac{D(\boldsymbol{Y}; \hat{\boldsymbol{\mu}}_{\text{null}}) - D(\boldsymbol{Y}; \hat{\boldsymbol{\mu}})}{\hat{\phi}} \mathrel{\dot\sim} \chi^2_{p-1}.$$

If the H_0 is not rejected, it means all the **covariates** are regarded as **irrelevant**.

Pearson X^2 statistic

- The deviance is a **log-likelihood ratio** test between a given model and the saturated model, rescaled by ϕ.
- Hence, we may consider another test, like the **Rao-Score**, to obtain an alternative definition.

> Let W_u be the **Rao-Score** test comparing model M with the **saturated model**. Then, it holds:
>
> $$\phi W_u = X^2 = \sum_{i=1}^{n} \omega_i \frac{(y_i - \hat{\mu}_i)^2}{v(\hat{\mu}_i)},$$
>
> which is known as generalized **Pearson chi-squared statistic**.

- Karl Pearson introduced X^2 in 1900 for testing various hypotheses using the chi-squared distribution, such as the hypothesis of independence in contingency tables.
- Since W_u and W are **asymptotically equivalent**, so will be the chi-squared statistic X^2 and the deviance $D(\boldsymbol{Y}; \hat{\boldsymbol{\mu}})$ for large values of n.

Deviance of a Gaussian linear model

- In the classical **Gaussian linear model**, we have that $\theta_i = \mu_i$ and $b(\theta_i) = \theta_i^2/2$. Thus $\theta(y_i) = y_i$ and

$$
\begin{aligned}
D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) &= 2\sum_{i=1}^n \omega_i \left\{ y_i[\theta(y_i) - \theta(\hat{\mu}_i)] - [b(\theta(y_i)) - b(\theta(\hat{\mu}_i))] \right\} \\
&= 2\sum_{i=1}^n \{ y_i(y_i - \hat{\mu}_i) - y_i^2/2 + \hat{\mu}_i^2/2 \} \\
&= \sum_{i=1}^n (y_i^2 - 2y_i\hat{\mu}_i + \hat{\mu}_i^2) = \sum_{i=1}^n (y_i - \hat{\mu}_i)^2.
\end{aligned}
$$

- In the Gaussian case, the deviance is the **residuals sum of squares** and $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) = X^2$.

- Note that the **null deviance** is obtained with $\hat{\boldsymbol{\mu}}_{\text{null}} = (\bar{y}, \dots, \bar{y})$ so that

$$
D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}_{\text{null}}) = \sum_{i=1}^n (y_i - \bar{y})^2,
$$

namely the so-called **total deviance**.

Deviance of a Poisson model

- Let us consider a **Poisson regression** model, that is $\theta_i = \log \mu_i$ and $b(\theta_i) = \exp(\theta_i) = \mu_i$. Then $\theta(y_i) = \log y_i$ and

$$
\begin{aligned}
D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) &= 2 \sum_{i=1}^{n} \{y_i(\log y_i - \log \hat{\mu}_i) - y_i + \hat{\mu}_i\} \\
&= 2 \sum_{i=1}^{n} \{y_i \log(y_i/\hat{\mu}_i) - y_i + \hat{\mu}_i\},
\end{aligned}
$$

  with the **convention** that $y_i \log(y_i/\hat{\mu}_i) = 0$ whenever $y_i = 0$.

- The X^2 statistic in this case has a very simple form

$$
X^2 = \sum_{i=1}^{n} \frac{(y_i - \hat{\mu}_i)^2}{\hat{\mu}_i} = \sum_{i=1}^{n} \frac{(\text{observed}_i - \text{fitted}_i)^2}{\text{fitted}_i}.
$$

  As discussed in Salvan et al. (2020), Example 2.12, this can be seen as a **quadratic approximation** of the **deviance**, which is valid for large values of n.

Deviance of a binomial model I

- Let us consider a **Binomial regression** model $m_i Y_i = S_i \sim \text{Bimonial}(m_i, \pi_i)$ with $\mu_i = \pi_i$. Then

$$\ell_{\mathcal{M}}(\hat{\boldsymbol{\mu}}) = \sum_{i=1}^{n} \{m_i y_i \log(\hat{\mu}_i) + m_i(1 - y_i)\log(1 - \hat{\mu}_i)\}.$$

Therefore, under the convention $x\log(x) = 0$ as before, the deviance is

$$\begin{aligned} D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) &= 2\sum_{i=1}^{n} m_i \left\{ y_i \log\left(\frac{y_i}{\hat{\mu}_i}\right) + (1 - y_i)\log\left(\frac{1 - y_i}{1 - \hat{\mu}_i}\right)\right\} \\ &= 2\sum_{i=1}^{n} \left\{ m_i y_i \log\left(\frac{m_i y_i}{m_i\hat{\mu}_i}\right) + (m_i - m_i y_i)\log\left(\frac{m_i - m_i y_i}{m_i - m_i\hat{\mu}_i}\right)\right\}. \end{aligned}$$

- The quantities $m_i y_i$ and $m_i - m_i y_i$ can be interpreted as the number of observed **successes** and **failures**, respectively. Similarly, $m_i\hat{\mu}_i$ and $m_i - m_i\hat{\mu}_i$ represent their **predictions**. Hence, we can write

$$D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) = 2\sum_{j=1}^{2n} \text{observed}_j \log\left(\frac{\text{observed}_j}{\text{fitted}_j}\right)$$

Deviance of a binomial model II

- The X^2 statistic of a binomial model, recalling that $v(\mu_i) = \mu_i(1-\mu_i)$, equals to

$$X^2 = \sum_{i=1}^n \frac{(y_i - \hat{\mu}_i)^2}{\hat{\mu}_i(1-\hat{\mu}_i)/m_i} = \sum_{i=1}^n \frac{(m_i y_i - m_i\hat{\mu}_i)^2}{m_i\hat{\mu}_i} + \sum_{i=1}^n \frac{[(m_i - m_i y_i) - (m_i - m_i\hat{\mu}_i)]^2}{m_i - m_i\hat{\mu}_i}.$$

  The second representation follows after some **algebra**.

- The second equation shows that we can write

$$X^2 = \sum_{j=1}^{2n} \frac{(\text{observed}_j - \text{fitted}_j)^2}{\text{fitted}_j}.$$

- As already mentioned, the X^2 statistic can be seen as a **quadratic approximation** of the **deviance**.

Deviance as goodness of fit measure I

- The deviance is useful a **descriptive measure** for the **goodness of fit**.
- It is **tempting** to use the deviance as a formal **statistical test**, to verify if the current model is adequate compared to the saturated model.

- Suppose ϕ were **known**, then in the Gaussian case we would have $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}})/\phi \sim \chi^2_{n-p}$, which would allow us to check the adequacy of the model.
- Unfortunately, whenever $\hat{\phi}$ is **estimated** we obtain $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}})/\hat{\phi} \approx n - p$, and exactly $n - p$ in the Gaussian case, so this strategy can not be used.

- On the other hand, for example in Poisson e binomial regression, we have $\phi = 1$. Hence, the intuition tells us that, at least approximately, we should have

$$D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) \dot{\sim} \chi^2_{n-p}.$$

- Unfortunately, this is **not** the **case**: the saturated model is an "irregular case" in that the number of parameters $p = n$ grows with the sample size.
- The usual "large n" approximation does not hold in general, e.g. because χ^2_{n-p} itself depends on n.

Deviance as goodness of fit measure II

- Despite these bad news, it turns out that in some special cases, the χ^2_{n-p} approximation is still valid even for fixed values of n.

Then the **deviance** $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}})$ and the X^2 **Pearson statistic** are approximately distributed as a χ^2_{n-p} in the following cases:

- In binomial regression, for large values of m_i (small-dispersion asymptotics);
- In Poisson regression, for large values of the estimated means $\hat{\mu}_i$ (say $\hat{\mu}_i \geq 5$);
- When ϕ is known and $\phi \to 0$ (small-dispersion asymptotics).

- **Small-dispersion asymptotics** describe an alternative limiting regime in which the variance of the observations tends to 0.
- In binomial regression the X^2 statistic converges to χ^2_{n-p} more quickly than the deviance and has a **more trustworthy** p-value when some expected success or failure totals are less than about five.
- The χ^2_{n-p} approximation is **very poor** for binary regression, i.e. when $m_i = 1$.

On pseudo-R^2

- There exist several generalizations of the R^2 statistic for linear models, called **pseudo-R^2** (e.g. McFadden, Cox & Snell, Nagelkerke, Tjur, etc.).
- These indices are **difficult to interpret** and could mislead those accustomed with standard R^2. A pseudo-$R^2 \approx 0.4$ may indicate a nearly perfect fit (i.e. `Beetles` data), which is confusing.
- On top of this, these pseudo-R^2 produce different answers depending on the **aggregation** of the data.
- The recommendation is to rely on indices tailored for the data at hand, such as the ROC curve for binary data, or the correlation between $\boldsymbol{y}$ and $\hat{\boldsymbol{\mu}}$.
- The residual **deviance** is also a useful tool, especially for comparing models.
- Pseudo-R^2 are often shown by default in other software, such as SAS or SPSS.

Example: Beetles data, output of summary

- This is how the summary of a GLM looks like. It is very similar to the summary of lm. At this stage of the course, you should be able to understand almost everything.

```
Call:
glm(formula = cbind(deaths, m - deaths) ~ logdose, family = "binomial",
    data = Beetles)

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  -60.717      5.181  -11.72   <2e-16 ***
logdose       34.270      2.912   11.77   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 284.202  on 7  degrees of freedom
Residual deviance:  11.232  on 6  degrees of freedom
AIC: 41.43

Number of Fisher Scoring iterations: 4
```

- Null deviance corresponds to the **null deviance** $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}_{\text{null}})$.
- Residual deviance corresponds to the **deviance** $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}})$ of the current model.

Example: Beetles data, output of anova

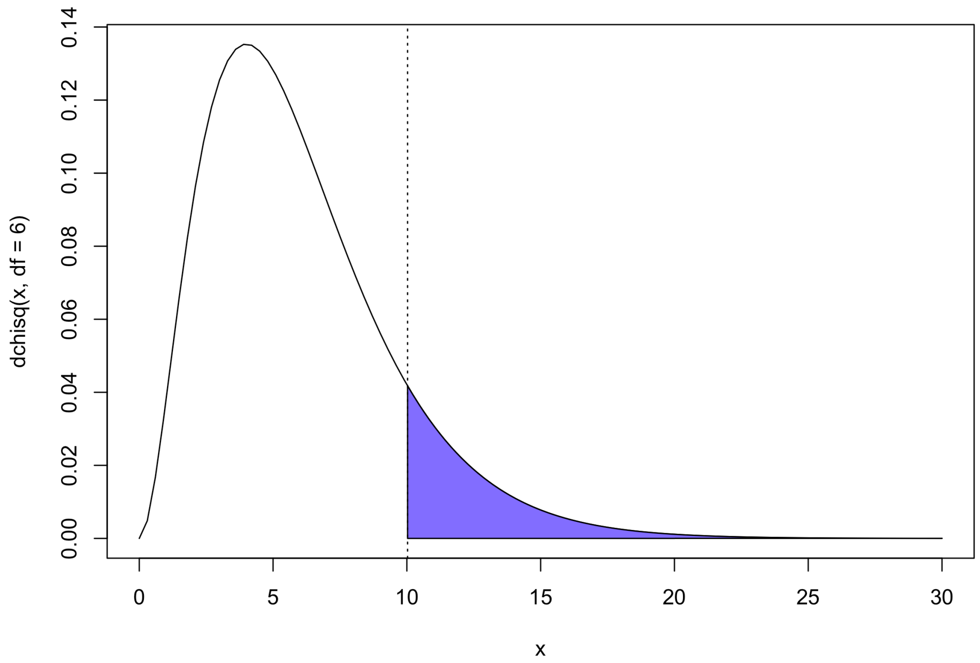
- anova(model0, model1) computes **log-likelihood ratio test** comparing two nested models: the **reduced** model M_0 with p_0 parameters and the **full** model M_1 with p parameters.

```
Analysis of Deviance Table

Model 1: cbind(deaths, m - deaths) ~ 1
Model 2: cbind(deaths, m - deaths) ~ logdose
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1         7    284.202
2         6     11.232  1   272.97 < 2.2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

- Resid Df are the **degrees of freedom** of the **deviances**, that is $n - p_0$ and $n - p$, respectively.
- Resid. Dev are the **deviances** of the **reduced** model $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}_0)$ and the **full** model $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}})$. In this example, the reduced model is also the **null model**.
- Df refers to the **degrees of freedom** $q = p - p_0$ of the test, which is $q = 1$ in this case.
- Deviance indicates the **change in deviance**, that is $\phi W = D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}_0) - D(\boldsymbol{y}; \hat{\boldsymbol{\mu}})$.
- Pr(>Chi) is the **p-value** of the log-likelihood ratio test W.

Example: Beetles data, goodness of fit



- The **deviance** equals $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) = 11.232$, with $n - p = 8 - 2 = 6$ degrees of freedom. The observed X^2 **Pearson statistic** equals 10.027.
- Using the X^2 statistic with 6 degrees of freedom, we obtain the p-value $\mathbb{P}(X^2 > 10.027) = 0.124$, as pictured above, which can be interpreted as a **slight** lack of fit.

Example: `Aids` data, output of `summary`

- Below is shown the `summary` of the Poisson regression model with the `Aids` data.

```
Call:
glm(formula = deaths ~ period, family = "poisson", data = Aids)

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  0.30365    0.25387   1.196    0.232
period       0.25896    0.02224  11.645   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 208.754  on 13  degrees of freedom
Residual deviance:  30.203  on 12  degrees of freedom
AIC: 86.949

Number of Fisher Scoring iterations: 5
```

Example: `Aids` data, output of `anova` and `lrtest`

```
Analysis of Deviance Table

Model 1: deaths ~ 1
Model 2: deaths ~ period
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1        13    208.754
2        12     30.203  1   178.55 < 2.2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

> The use of the term `deviance` to indicate the **difference** between two deviances is a bit **misleading**.
> I do not know the the reason, but the `lrtest` function of the `lmtest` package changed it.

```
Likelihood ratio test

Model 1: deaths ~ 1
Model 2: deaths ~ period
  #Df   LogLik Df  Chisq Pr(>Chisq)
1   1 -130.750
2   2  -41.475  1 178.55  < 2.2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Example: Aids data, goodness of fit

- The **deviance** equals $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) = 30.203$, with $n - p = 14 - 2 = 12$ degrees of freedom. The observed X^2 **Pearson statistic** equals 29.92.
- Using the X^2 statistic with 12 degrees of freedom, we obtain the p-value $\mathbb{P}(X^2 > 29.92) = 0.0028$, therefore **rejecting** the hypothesis that this model has a comparable fit with the saturated model.
- The X^2 goodness of fit test indicates a potential issue with the model, but it does not explain **why**.
- A few remedies could be:
  a. Choosing a different **link function**;
  b. Including an **additional covariate** (if available), and/or considering non-linear **transformations** of the available ones;
  c. Choosing a different **distribution** instead of the Poisson, such as the negative binomial;
  d. Accounting for **overdispersion** using quasi-likelihoods, that is, estimating ϕ from the data rather than fixing it to $\phi = 1$.
- It turns out that selecting the link function $g(\mu_i) = \sqrt{\mu_i}$ yields a much better fit with $X^2 = 17.09$, whose p-value is 0.146. This is not the only possible solution.

Residuals

- Linear models have an additive structure $y_i = \boldsymbol{x}_i^T \beta + \epsilon_i$ therefore the residuals can be estimated as

$$r_i = y_i - \hat{\mu}_i.$$

  We call these the **response residuals**.

- GLMs do not have an additive decomposition, therefore we need define a good **generalization** of **residuals**. There are at least 2 alternatives: Pearson and deviance residuals.
- Ideally, we would like residuals to have approximately 0 mean and unitary variance, but these properties will not hold exactly.

- The analysis of the residuals is very helpful for identifying any misspecification as well as hinting the solution. In particular, it is useful for instance to:
  a. Choosing the correct variance function $v(\mu_i)$, i.e. the correct response distribution;
  b. Choosing the correct link function;
  c. Identifying latent patterns, often an indication of an omitted variable;
  d. Identifying potential outliers and leverage points.

Pearson residuals

For a GLM with variance function $v(\mu_i)$, we call **Pearson residuals** the following quantities:

$$r_{i,P} = \frac{y_i - \hat{\mu}_i}{\sqrt{v(\hat{\mu}_i)/\omega_i}}, \qquad i = 1, \dots, n.$$

- Pearson residuals rescale the response residuals, accounting for **heteroschedasticity**.
- Pearson residuals own their name to the fact that the X^2 statistic is obtained as

$$X^2 = \sum_{i=1}^{n} r_{i,P}^2 = \sum_{i=1}^{n} \omega_i \frac{(y_i - \hat{\mu}_i)^2}{v(\mu_i)}.$$

Moreover, the dispersion parameter, when present, can be estimated as

$$\hat{\phi} = \frac{1}{n-p} \sum_{i=1}^{n} r_{i,P}^2.$$

Deviance residuals

The deviance of a GLM can be written as a sum of individual contributions $D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) = \sum_{i=1}^n d_i$ and

$$d_i = 2\omega_i \left\{ y_i[\theta(y_i) - \theta(\hat{\mu}_i)] - [b(\theta(y_i)) - b(\theta(\hat{\mu}_i))] \right\}, \qquad i = 1, \dots, n.$$

We call **deviance residuals** the following quantities:

$$r_{i,D} = \text{sign}(y_i - \hat{\mu}_i)\sqrt{d_i}, \qquad i = 1, \dots, n.$$

- By definition, the deviance is obtained as

$$D(\boldsymbol{y}; \hat{\boldsymbol{\mu}}) = \sum_{i=1}^n r_{i,D}^2.$$

- Deviance residuals are the **default** choice in the `residuals` **R** function.
- Pearson residuals are an asymptotic approximation of deviance residuals, therefore these two quantities are often very similar in practice.

A weighted projection matrix

- In linear models, we considered the **hat matrix** $\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T$, whose diagonal elements h_i are called **leverages** and it holds $\text{var}(r_i) = \sigma^2(1 - h_i)$.

- Several arguments can be invoked to justify the following **weighted hat matrix** in GLMs
$$\boldsymbol{H}_W = \boldsymbol{W}^{1/2}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{W}\boldsymbol{X})^{-1}\boldsymbol{X}\boldsymbol{W}^{1/2}.$$
This matrix is **symmetric** ($\boldsymbol{H}_W = \boldsymbol{H}_W^T$) and **idempotent** ($\boldsymbol{H}_W^2 = \boldsymbol{H}_W$), i.e. a projection matrix.

- We denote with $h_{i,W}$ the diagonal elements of $\boldsymbol{H}_W$, which are the **leverages** of a GLM. In practice $\boldsymbol{W}$ is estimated from the data, therefore the leverages will depend on the **response**.

- It can be shown, as in Agresti (2015), Section 4.4.5, that
$$\text{var}(y_i - \hat{\mu}_i) \approx \phi/\omega_i v(\mu_i)(1 - h_{i,W}) \quad \implies \quad \text{var}(r_{i,P}) \approx \phi(1 - h_{i,W}).$$

- A technical but deeper discussion about $\boldsymbol{H}_W$ can be found in the Appendix of Chapter 4 of Agresti (2015), where stronger analogies with linear models are shown.

Standardized residuals

- In analogy of what has been done for GLMs, we can consider the **standardized** version of Pearson and deviance residuals.
- **Standardized Pearson residuals** are defined as

$$\tilde{r}_{i,P} = \frac{r_{i,P}}{\sqrt{\hat{\phi}(1-\hat{h}_{i,W})}} = \frac{y_i - \hat{\mu}_i}{\sqrt{\hat{\phi}/\omega_i v(\hat{\mu}_i)(1-\hat{h}_{i,W})}}, \qquad i = 1, \dots, n,$$

  where $\hat{\phi}$ is an estimate of ϕ (if unknown) and $\hat{h}_{i,W}$ is an estimate of the leverages.
- **Standardized deviance residuals** are defined as

$$\tilde{r}_{i,D} = \frac{r_{i,D}}{\sqrt{\hat{\phi}(1-\hat{h}_{i,W})}}, \qquad i = 1, \dots, n.$$

- We can also obtain an **approximate Cook's distance** by considering

$$c_i = \tilde{r}_{i,P}^2 \frac{\hat{h}_{i,W}}{p(1-\hat{h}_{i,W})}, \qquad i = 1, \dots, n.$$

On Q-Q plots and other practicalities

- It is sometimes recommended to check the normality of the Pearson/deviance residuals using Q-Q plots. Such a plot is also provided in **R**.
- Indeed, for example under small dispersion asymptotics or other specific, Pearson residuals are **approximately** Gaussian.
- However, these conditions are often not met. For example, in binary data the response $y_i \in \{0, 1\}$ can only assume two values and the residuals will not be Gaussian distributed, even for large n.
- Actually, the analysis for the residuals in **binary data** do **not provide useful information**; see e.g. Salvan et al. (2020), Section 3.6.

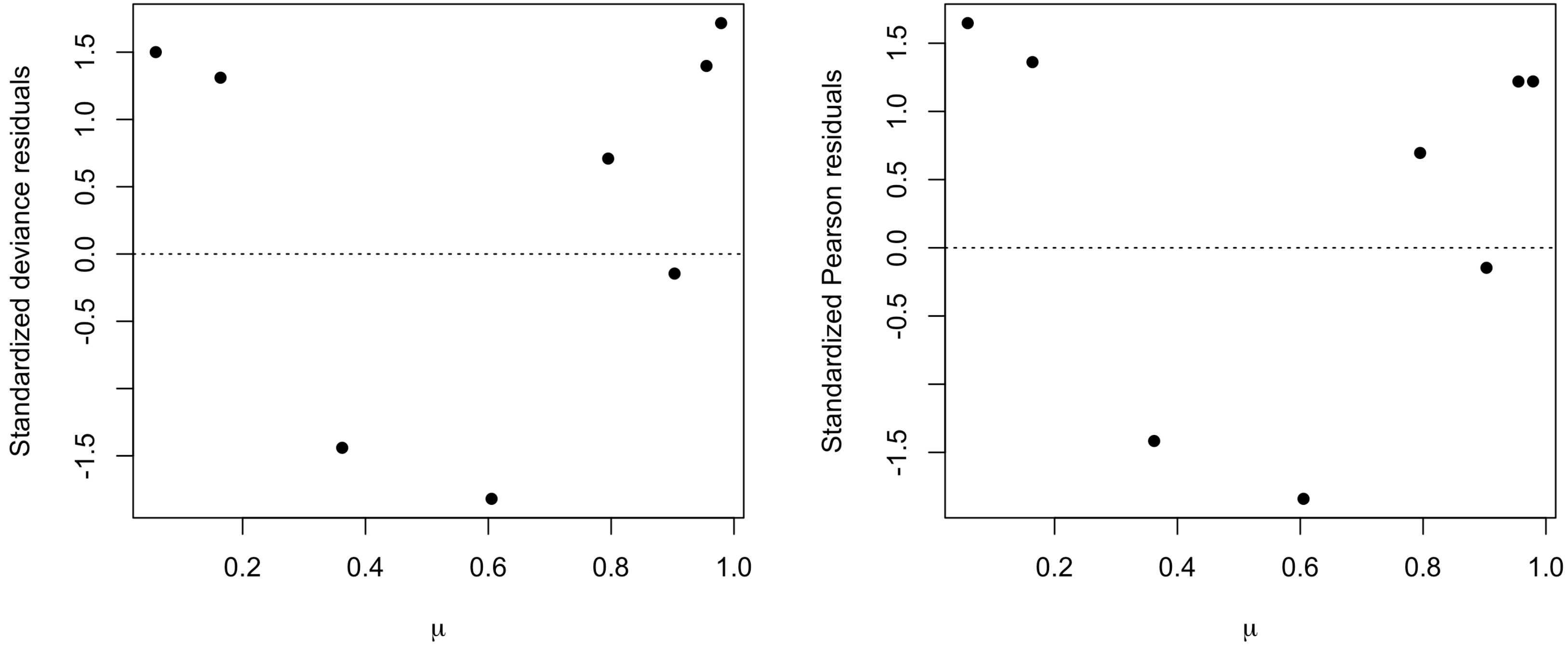
> The analysis of residuals in GLMs is often useful but should be taken *cum grano salis*, particularly when dealing with discrete responses that take only a few distinct values.
>
> Overreliance on residual analysis can encourage automatic decisions rather than thoughtful, critical judgment. A good model should not be discarded solely on the basis of a "bad" diagnostic plot.

On identifying and removing outliers

- The analysis of the residuals can also help in identifying outliers and influence points. However, we must be careful in drawing conclusions.
- An outlier might be detected as such simply as the consequence of **model misspecification**, e.g. an omitted variable.
- In the vast majority of cases, the presence of outliers should be carefully dealt with by carefully modifying the model.
- There are instances in which outliers are actually **contaminated data points** (e.g. `age = -3`). If there is strong and contextual evidence that this might be the case, then these points should be **removed**. Otherwise, removing data points is a **bad practice**.

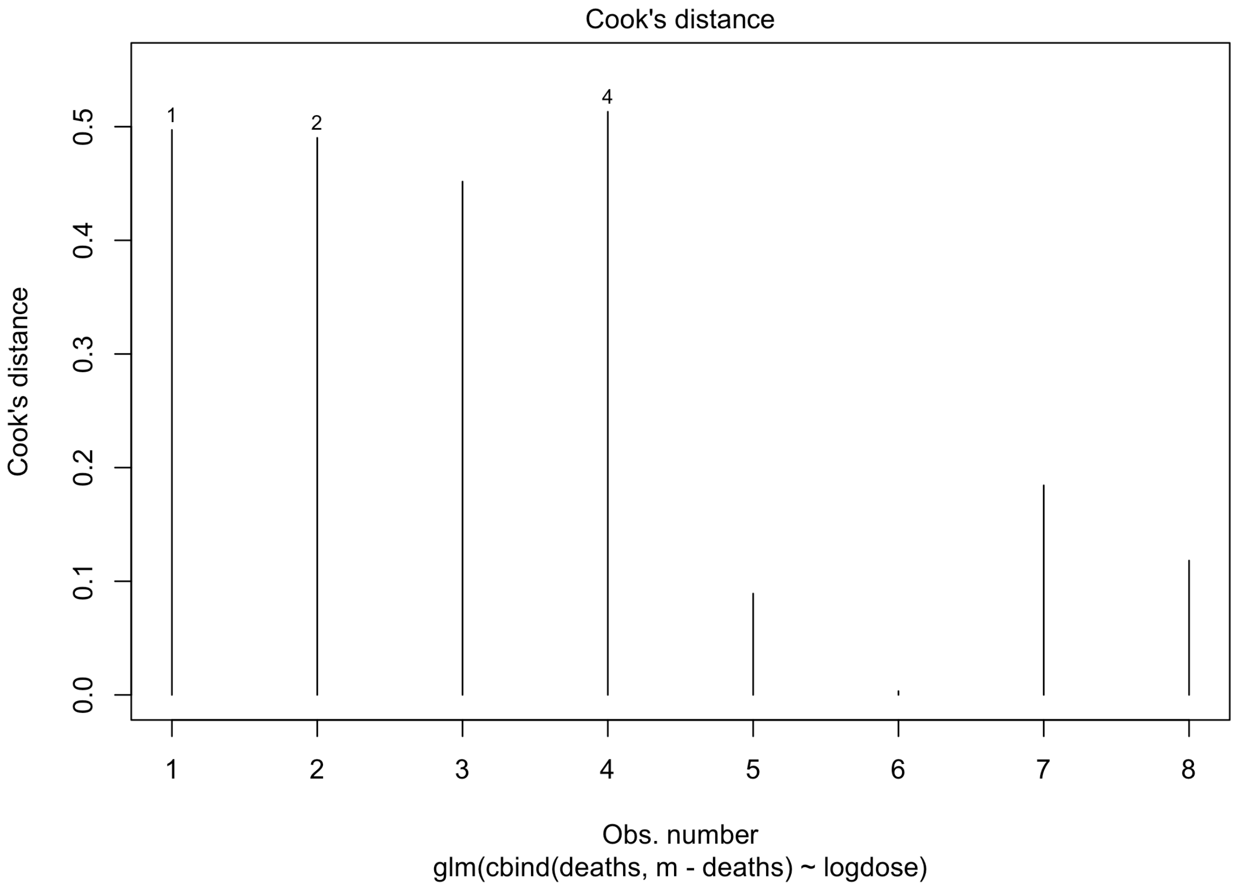
> In statistical modelling, we wish to find a model that fits our data, not a dataset that is aligned with our prescribed model.
>
> Discarding observations until the hypoteshes are reasonable it skews the overall analysis and does not answer any meaningful scientific or business question.

Example: Beetles data



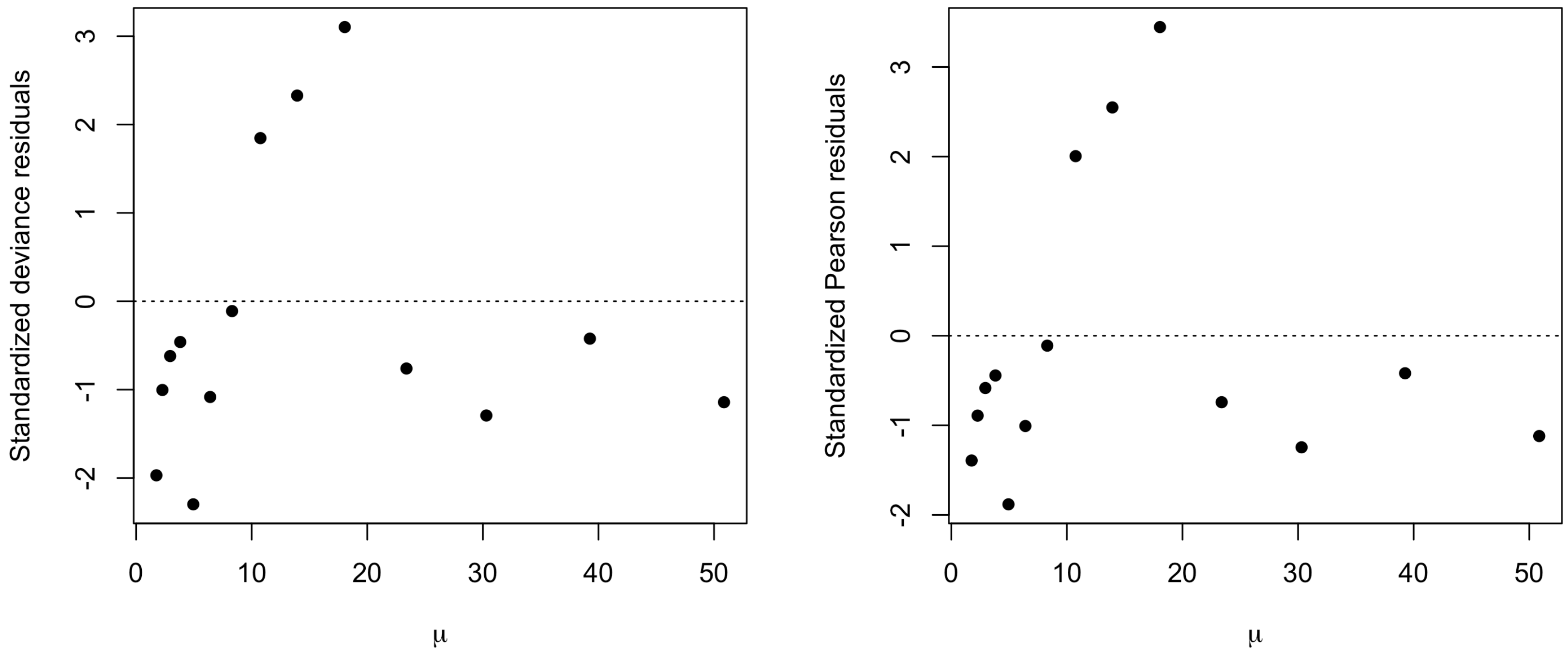
- A formal test already confirmed that there are **no** noticeable **differences** between this model and the saturated model. The analysis of the residuals confirms it.
- Deviance residuals and Pearson residuals are very similar, as expected.

Example: Beetles data



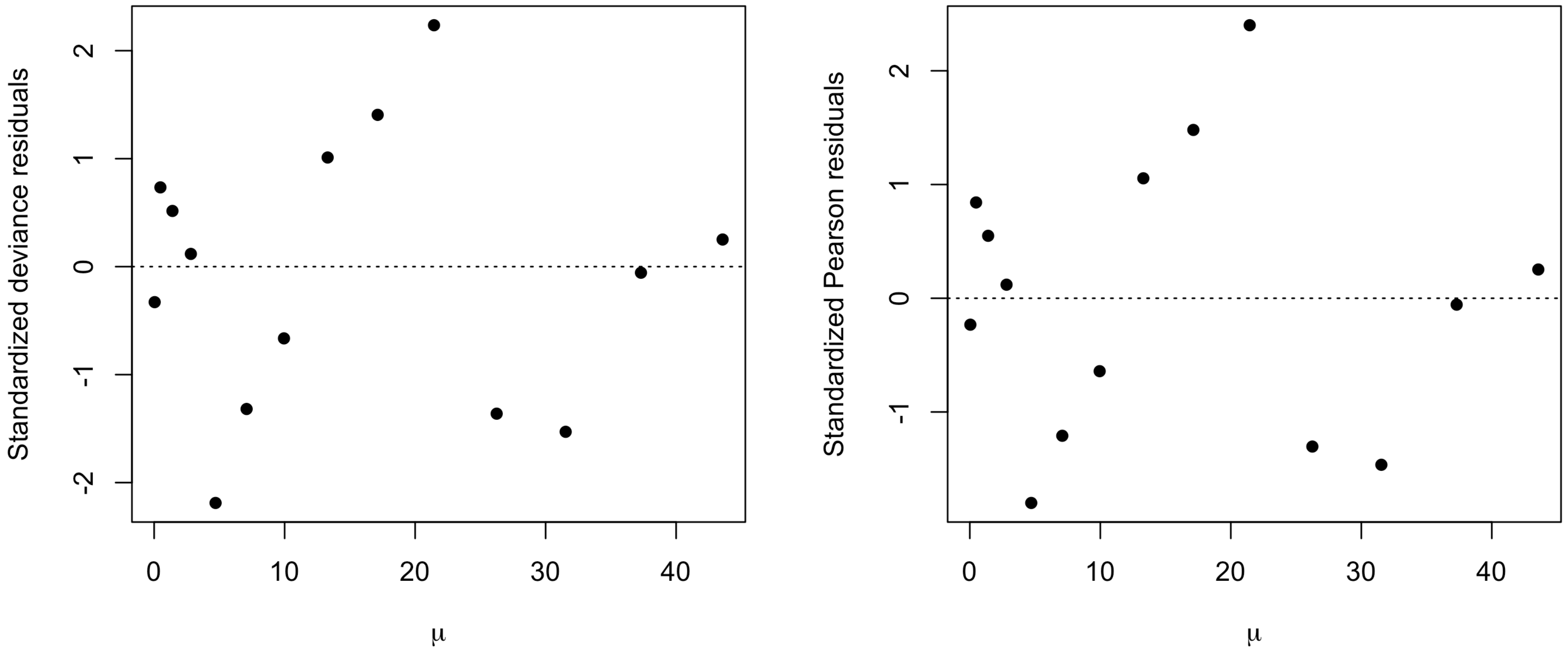
- The Cook's distance also confirms that there are not strong influence points.

Example: Aids data



- From both residuals plots it is evident that three observations are highly underestimated, while the others are slightly underestimated.
- The lack of fit can be solved, in this case, by using a different link function.

Example: Aids data



- We estimated a Poisson regression model with a **non-canonical link** function $g(\mu_i) = \sqrt{\mu_i}$.
- This yields a much **better fit**, as we previously discussed. The residuals are also better behaved.

Model selection

Model selection process

- **Model selection** for GLMs faces the same issues as for linear models.
- The selection process becomes more difficult as the number of explanatory variables p increases, because of the growth in possible effects and interactions. There are two competing goals:
  a. The model should be complex enough to **fit the data well**;
  b. On the other hand, it should **smooth rather than overfit** the data and ideally remain **simple to interpret**.
- Most research studies are designed to answer certain questions, which guide the choice.
- **Confirmatory analyses** use a restricted set of models, e.g. for testing a study hypothesis about an effect by comparing models **with and without** that effect.
- **Exploratory studies**, instead, search among possible models which may provide clues about the structure of effects or can raise questions for future research.
- In either case, it is helpful first to study the **marginal effect** of each predictor. Use **descriptive statistics** and a scatterplot matrix to get a feel for those effects.

Automatic model selection

- With p **explanatory variables**, the number of potential models is the huge number

$$\sum_{k=1}^{p} \binom{p}{k} = 2^p.$$

- **Best subset selection** identifies the model that optimizes an **information criterion** e.g. AIC or BIC, which are defined as

$$\text{AIC} = -2\ell(\hat{\beta}) + 2k, \qquad \text{BIC} = -2\ell(\hat{\beta}) + k \log n,$$

  where k is the number of parameters in the model.

- Best subset selection is **computationally intensive** when p is large, to the extent that it is not even feasible in most cases, but approximations such as **forward** and **backward** selection are possible.

- In **exploratory studies**, these methods are useful if applied **cautiously**.

- As we shall discuss, an excess of automatism may lead to good predictive performance, but it may fail in making the model simple or interpretable.

Stepwise procedures: forward and backward selection

- **Forward selection** adds terms sequentially. At each stage it selects the term giving the greatest improvement in terms of **deviance** or other goodness of fit measures.
- The process stops when further additions do not improve the it, according to statistical significance (i.e. a log-likelihood ratio test) or a criterion for judging the model fit (such as the AIC or BIC).
- A stepwise variation of this procedure rechecks, at each stage, whether terms added at previous stages are still needed.

- **Backward elimination** begins with a complex model and sequentially removes terms.
- At each stage, it selects the term whose removal has the least damaging effect on the model, such as the largest p-value in a test or the least deterioration in a criterion for judging the model fit.
- The process stops when any further deletion leads to a poorer it.

> Whenever possible, i.e. when p is not too large, we recommend **manually** performing each stage of forward or backward procedures and **avoid fully automatic procedures**.

Comments on forward/backward selection I

- An **interaction term** should not be included without its **main effects**.
- For **qualitative predictors** with > 2 categories: add/drop the **entire variable**, not just one indicator. Otherwise, results depend on the reference category used in coding.

- Some statisticians prefer **backward elimination** over **forward selection**. It is safer to delete terms from an overly complex model than to **add** to an overly simple one.
- Forward selection based on significance tests:
  a. May stop prematurely if a test has **low power**.
  b. Early-stage comparisons often involve **inadequate models**, making tests **questionable**.

- Neither backward nor forward strategies guarantee a **meaningful model**.
- Evaluating many terms increases risk of **chance findings**. If true effects are **weak**, the largest sample effect likely **overestimates** the truth.

- Use of standard significance tests in selection lacks **theoretical justification**. Distribution of minimum or maximum p-values at each stage is not the same as the distribution of a **pre-selected variable**. This issue is called **multiple testing** and leads to **overconfident** conclusions.

Comments on forward/backward selection II

- Statistical significance is not the same as **practical significance**; do not rely only on significance tests.
- The price to pay for adding an irrelevant variable is an increase in **variance** of the estimates. The price to pay for dropping a relevant variable is an increase in **bias**.
- It is possible to include variables central to the study goals even if **not significant**:
  - It enables comparisons with other studies where the effect is significant, perhaps because of a larger sample size;
  - If the variable is a potential **confounder**, i.e. possibly relevant for predicting the response, but not of direct interest, including it in the model may help to reduce bias in estimating relevant effects of key explanatory variables.
- Do not keep variables just because they are **significant**.
  - As an example, consider an adjusted $R^2 = 0.39$ in a linear model with interactions vs. 0.38 without. The simpler model may be preferable being more interpretable.
- Algorithmic selection methods are no substitute for careful thought in model building.

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