NMST432 Advanced Regression Models

Extended Course Notes

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These course notes contain the whole contents of the course "NMST432 Advanced regression models", which is a part of the curriculum of the Master's program "Probability, Mathematical Statistics and Econometrics".

This document undergoes continuing development. The author will appreciate notifications by the reader of potential typos or misprints.

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1. Review of Linear Regression

1.1. Definition and Assumptions

Consider n independent copies of random vectors $(Y_i, \boldsymbol{X}_i)$, $i = 1, \ldots, n$. Each $\boldsymbol{X}_i$ has $p < n$ components $(X_{i1}, \ldots, X_{ip})$.

Note.

- Y_i is called *the response*[*]. The components of $\boldsymbol{X}_i$ are called *covariates* (explanatory variables, predictors, regressors)[†].
- The covariate X_{i1} is usually taken as 1.
- In certain applications, the covariates can be fixed quantities rather than random variables. Throughout this course, we will consider covariates random. Extensions to fixed covariates usually hold with some additional conditions but the proofs require more effort.

Notation. Let $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\mathsf{T}$ and

$$\mathbb{X} = \begin{pmatrix} \boldsymbol{X}_1^\mathsf{T} \\ \boldsymbol{X}_2^\mathsf{T} \\ \vdots \\ \boldsymbol{X}_n^\mathsf{T} \end{pmatrix}.$$

The n by p matrix $\mathbb{X}$ is called *the regression matrix*[‡]. We assume $r(\mathbb{X}) = p$ (full rank).

Definition 1.1. The data $(Y_i, \boldsymbol{X}_i)$ satisfy the linear regression model if the response Y_i can be written as

$$Y_i = \boldsymbol{X}_i^\mathsf{T} \boldsymbol{\beta}_0 + \varepsilon_i,$$

where $\boldsymbol{\beta}_0 = (\beta_{01}, \ldots \beta_{0p})^\mathsf{T}$ is a vector of unknown *regression parameters (coefficients)*[§] and $\varepsilon_1, \ldots, \varepsilon_n$ are independent random variables such that $\mathsf{E}\left[\varepsilon_i \,\middle|\, \boldsymbol{X}_i\right] = 0$, and $\mathsf{var}\left[\varepsilon_i \,\middle|\, \boldsymbol{X}_i\right] = \sigma^2$.$\nabla$

Note. The unobserved random variables ε_i are called *error terms (disturbances)*[¶], σ^2 is called *residual variance*[‖].

[*] Česky *odezva* [†] Česky *regresory, nezávisle proměnné, vysvětlující veličiny, prediktory, kovariáty* [‡] Česky *regresní matice* [§] Česky *regresní koeficienty* [¶] Česky *chybové členy* [‖] Česky *residuální rozptyl*

Note. Another convenient formulation of the model is based on conditional moments and it avoids the expression of the error terms:

The linear regression model holds if and only if

- $Y_1, \dots, Y_n$ are independent
- $\mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i\right] = \boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}_0$
- $\mathsf{var}\left[Y_i \middle| \boldsymbol{X}_i\right] = \sigma^2$

Thus, the linear regression model specifies the first two conditional moments of Y_i given $\boldsymbol{X}_i$.

Note. We will use the notation E, var for the conditional expectation and variance, respectively, given $\boldsymbol{X}_i$. The symbol E_X will be used for unconditional expectation over the distribution of $\boldsymbol{X}_i$.

Note. The regression parameters express the influence of $\boldsymbol{X}_i$ on $\mathsf{E}\, Y_i$. Assuming that $X_{i1} = 1$, we have

$$\beta_{01} = \mathsf{E}\left[Y_i \middle| X_{i2} = 0, X_{i3} = 0, \dots, X_{ip} = 0\right]$$

and, with $\boldsymbol{e}_j = (0, \dots, 0, 1, 0, \dots, 0)^\mathsf{T}$ being a p-vector of zeros with 1 at the j-th position,

$$\beta_{0j} = \mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i = \boldsymbol{x} + \boldsymbol{e}_j\right] - \mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i = \boldsymbol{x}\right], \quad j = 2, \dots, p.$$

1.2. Estimation

The regression coefficients $\boldsymbol{\beta}_0$ are estimated by *the least squares estimator* (LSE) $\widehat{\boldsymbol{\beta}}$ that minimizes the sum of squares

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^p} \sum_{i=1}^n (Y_i - \boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta})^2 = \arg\min_{\boldsymbol{\beta}\in\mathbb{R}^p} (\boldsymbol{Y} - \mathbb{X}\boldsymbol{\beta})^\mathsf{T}(\boldsymbol{Y} - \mathbb{X}\boldsymbol{\beta}),$$

i.e., solves the system of *normal equations*

$$\sum_{i=1}^n \boldsymbol{X}_i(Y_i - \boldsymbol{X}_i^\mathsf{T}\widehat{\boldsymbol{\beta}}) = \boldsymbol{0}.$$

Because $\mathbb{X}$ is of full rank, the single solution to the system is

$$\widehat{\boldsymbol{\beta}} = (\mathbb{X}^\mathsf{T}\mathbb{X})^{-1}\mathbb{X}^\mathsf{T}\boldsymbol{Y}.$$

Note.

- $\mathsf{E}\,\widehat{\boldsymbol{\beta}} = \boldsymbol{\beta}_0$ (unbiased), $\mathsf{var}\,\widehat{\boldsymbol{\beta}} = \sigma^2(\mathbb{X}^\mathsf{T}\mathbb{X})^{-1}$.
- The vector
$$\widehat{\boldsymbol{Y}} = \mathbb{X}\widehat{\boldsymbol{\beta}} = \mathbb{X}(\mathbb{X}^\mathsf{T}\mathbb{X})^{-1}\mathbb{X}^\mathsf{T}\boldsymbol{Y} = \mathbb{H}\boldsymbol{Y}$$
is called *the vector of fitted values*[*].

[*] Česky *vektor odhadnutých (vyrovnaných) hodnot*

- The projection matrix $\mathbb{H} \stackrel{\text{df}}{=} \mathbb{X}(\mathbb{X}^\mathsf{T}\mathbb{X})^{-1}\mathbb{X}^\mathsf{T}$ is idempotent, with rank p. It satisfies $\mathbb{H}\mathbb{X} = \mathbb{X}$. The matrix $\mathbb{I}_n - \mathbb{H}$ is also idempotent with rank $n-p$, and satisfies $(\mathbb{I}_n - \mathbb{H})\mathbb{X} = \mathbf{0}$.
- $\mathsf{E}\,\widehat{\boldsymbol{Y}} = \mathbb{X}\boldsymbol{\beta}_0$, $\mathsf{var}\,\widehat{\boldsymbol{Y}} = \sigma^2\mathbb{H}$.
- The random vector $\boldsymbol{u} \stackrel{\text{df}}{=} \boldsymbol{Y} - \widehat{\boldsymbol{Y}} = (\mathbb{I}_n - \mathbb{H})\boldsymbol{Y}$ is called *the vector of residuals**. It satisfies $\mathsf{E}\,\boldsymbol{u} = \mathbf{0}$, $\mathsf{var}\,\boldsymbol{u} = \sigma^2(\mathbb{I}_n - \mathbb{H})$.
- The random variable

$$SS_e \stackrel{\text{df}}{=} \boldsymbol{u}^\mathsf{T}\boldsymbol{u} = \sum_{i=1}^{n}(Y_i - \boldsymbol{X}_i^\mathsf{T}\widehat{\boldsymbol{\beta}})^2 = \boldsymbol{Y}^\mathsf{T}(\mathbb{I}_n - \mathbb{H})\boldsymbol{Y}$$

  is called the *residual sum of squares*†. Because $\mathsf{E}\,SS_e = (n-p)\sigma^2$, we obtain an unbiased estimator of residual variance as $\widehat{\sigma}^2 = SS_e/(n-p)$.

1.3. Normal Linear Regression

For normally distributed errors, additional useful properties can be derived. Assume now that $\boldsymbol{\varepsilon} \sim \mathsf{N}_n(\mathbf{0}, \sigma^2\mathbb{I}_n)$.

Proposition 1.1. *Under normality,*

(i) $\boldsymbol{Y} \sim N_n(\mathbb{X}\boldsymbol{\beta}_0, \sigma^2\mathbb{I}_n)$

(ii) $\widehat{\boldsymbol{\beta}} \sim N_p(\boldsymbol{\beta}_0, \sigma^2(\mathbb{X}^T\mathbb{X})^{-1})$

(iii) $\widehat{\boldsymbol{Y}} \sim N_n(\mathbb{X}\boldsymbol{\beta}_0, \sigma^2\mathbb{H})$

(iv) $\boldsymbol{u} \sim N_n(\mathbf{0}, \sigma^2(\mathbb{I}_n - \mathbb{H}))$

(v) $SS_e/\sigma^2 \sim \chi^2_{n-p}$

(vi) $\widehat{\boldsymbol{\beta}}$ *and* SS_e *are independent*

(vii) Let $\boldsymbol{c}$ *be any non-zero* p*-vector of real constants. Then*

$$\frac{\boldsymbol{c}^T\widehat{\boldsymbol{\beta}} - \boldsymbol{c}^T\boldsymbol{\beta}_0}{\sqrt{\widehat{\sigma}^2\boldsymbol{c}^T(\mathbb{X}^T\mathbb{X})^{-1}\boldsymbol{c}}} \sim t_{n-p}$$

(viii) Assume the model $\boldsymbol{Y} = \mathbb{X}\boldsymbol{\beta}_0 + \boldsymbol{\varepsilon}$*, where* $\mathbb{X} = (\mathbb{X}_A|\mathbb{X}_B)$ *and* $\boldsymbol{\beta}_0 = (\boldsymbol{\beta}_A^T, \boldsymbol{\beta}_B^T)^T$*,* $\boldsymbol{\beta}_B \in \mathbb{R}_m$*,* $\boldsymbol{\beta}_A \in \mathbb{R}^{p-m}$*, and introduce the submodel* $\boldsymbol{Y} = \mathbb{X}_A\boldsymbol{\beta}_A + \boldsymbol{\varepsilon}'$*. Let* SS_e *and* SS_h *be the residual sums of squares in the model and submodel, respectively. If the submodel is true (*$H_0 : \boldsymbol{\beta}_B = 0$ *holds) then*

$$F = \frac{n-p}{m}\,\frac{SS_h - SS_e}{SS_e} \sim F_{m,n-p}. \tag{1.1}$$

♢

It can be also shown that, under normality, $\widehat{\boldsymbol{\beta}}$ is the best linear unbiased estimator and the maximum likelihood estimator, so it possesses optimality properties.

* Česky *vektor residuí* † Česky *residuální součet čtverců*

1.4. Asymptotic Properties of the LSE

Let $(Y_i, \boldsymbol{X}_i)$, $i = 1, \dots, n$, be iid. Assume Definition 1.1 (without normality). Denote $\mathbb{D}_X = \mathsf{E}_X \boldsymbol{X}_i \boldsymbol{X}_i^\mathsf{T}$.

Proposition 1.2. *Let $\mathbb{D}_X$ be a finite regular matrix. Then*

(i) $\widehat{\boldsymbol{\beta}} \xrightarrow{P} \boldsymbol{\beta}_0$ *as* $n \to \infty$,

(ii) $\sqrt{n}(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) \xrightarrow{D} N_p(\mathbf{0}, \sigma^2 \mathbb{D}_X^{-1})$ *as* $n \to \infty$. ♢

Proposition 1.2(ii) is an asymptotic restatement of Proposition 1.1(ii). Other parts of Proposition 1.1 also hold asymptotically even if the data are not normal.

Now relax the assumption of equal variance: assume only $\mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i\right] = \boldsymbol{X}_i^\mathsf{T} \boldsymbol{\beta}_0$. Let $\mathsf{var}\left[Y_i \middle| \boldsymbol{X}_i\right] = \sigma^2(\boldsymbol{X}_i)$ be stochastically bounded (finite expectation follows). Denote $\mathbb{V}_X = \mathsf{E}_X \sigma^2(\boldsymbol{X}_i) \boldsymbol{X}_i \boldsymbol{X}_i^\mathsf{T}$.

Proposition 1.3. *Let $\mathbb{V}_X$ be finite and $\mathbb{D}_X$ be finite and regular. Then*

(i) $\widehat{\boldsymbol{\beta}} \xrightarrow{P} \boldsymbol{\beta}_0$ *as* $n \to \infty$,

(ii) $\sqrt{n}(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) \xrightarrow{D} N_p(\mathbf{0}, \mathbb{D}_X^{-1} \mathbb{V}_X \mathbb{D}_X^{-1})$ *as* $n \to \infty$. ♢

When equal variances hold, $\mathbb{V}_X = \sigma^2 \mathbb{D}_X$ and the result in Proposition 1.3(ii) transforms into the result in Proposition 1.2(ii).

Consistent estimates of $\mathbb{D}_X$ and $\mathbb{V}_X$ are

$$\widehat{\mathbb{D}}_n = \frac{1}{n} \mathbb{X}^\mathsf{T} \mathbb{X}$$

and

$$\widehat{\mathbb{V}}_n = \frac{1}{n} \mathbb{X}^\mathsf{T} \mathrm{diag}\,(u_i^2) \mathbb{X}.$$

So, if both normality and homoskedasticity are in doubt, one can use the OLS estimator $\widehat{\boldsymbol{\beta}}$ with variance

$$(\mathbb{X}^\mathsf{T}\mathbb{X})^{-1} \mathbb{X}^\mathsf{T} \mathrm{diag}\,(u_i^2) \mathbb{X} (\mathbb{X}^\mathsf{T}\mathbb{X})^{-1}$$

in place of the usual $\widehat{\sigma}^2 (\mathbb{X}^\mathsf{T}\mathbb{X})^{-1}$. This is called *the sandwich estimator*[*], or, in the econometric context, *White estimator*[†] (White 1980).

Many variants and improvements of this estimator have been proposed in the literature.

[*] Česky *sendvičový odhad* [†] Česky *Whiteův odhad*

1.5. Implications for Data Analysis

The asymptotic results we have just summarized indicate that linear regression model with ordinary least squares estimation of regression parameters can be used to obtain asymptotically correct statistical inference even if the response is not normal and the error terms do not have equal variance. We only need to have enough observations available for analysis so that the asymptotic results provide a reasonable approximation of the true distribution of the parameter estimator and other quantities of interest.

In this aspect, linear regression is actually a robust nonparametric statistical procedure.

(a) If the responses are *normal* and possess *equal variances* we can perform exact statistical inference based on Proposition 1.1 regardless of the size of the dataset (for any $n > p$).

(b) If the responses are *not normal* but have *equal variances* we can perform asymptotic inference based on Proposition 1.2 for large enough number of observations.

(c) If the responses are *not normal* and have *unequal variances* we can perform asymptotic inference based on Proposition 1.3 with sandwich variance estimator for large enough number of observations.

What number of observations is large enough to trust the asymptotic approaches (b) and (c) depends on the complexity of the linear model.

Furthermore, if the error variances are unequal but are known up to a proportionality constant, i.e., $\mathsf{var}\, Y_i = \sigma^2 w_i$ with known w_i, weighted least squares estimation can be used instead of the sandwich.

1.6. Interpretation with Transformed Response

Recall the linear model $\mathsf{E}\left[Y_i \,\middle|\, \boldsymbol{X}_i\right] = \boldsymbol{X}_i^{\mathsf{T}}\boldsymbol{\beta}_0$ with $\mathsf{var}\left[Y_i \,\middle|\, \boldsymbol{X}_i\right] = \sigma^2$. The regression parameters can be interpreted as

$$\beta_{01} = \mathsf{E}\left[Y_i \,\middle|\, X_{i2} = 0, X_{i3} = 0, \ldots, X_{ip} = 0\right]$$

and, $\boldsymbol{e}_j$ being the j-th unit vector of the length p,

$$\beta_{0j} = \mathsf{E}\left[Y_i \,\middle|\, \boldsymbol{X}_i = \boldsymbol{x} + \boldsymbol{e}_j\right] - \mathsf{E}\left[Y_i \,\middle|\, \boldsymbol{X}_i = \boldsymbol{x}\right].$$

When the response is non-normal, the common practice is to specify a linear model on a transformed response. Let g be some monotone function. The transformed model is

$$g(Y_i) = \boldsymbol{X}_i^{\mathsf{T}}\boldsymbol{\beta}_0 + \varepsilon_i$$

or $\mathsf{E}\left[g(Y_i) \,\middle|\, \boldsymbol{X}_i\right] = \boldsymbol{X}_i^{\mathsf{T}}\boldsymbol{\beta}_0$ with $\mathsf{var}\left[g(Y_i) \,\middle|\, \boldsymbol{X}_i\right] = \sigma^2$. The induced model for Y_i is

$$Y_i = g^{-1}(\boldsymbol{X}_i^{\mathsf{T}}\boldsymbol{\beta}_0 + \varepsilon_i).$$

In general, the effect of the covariates on $\mathsf{E}\, Y_i$ in this model cannot be expressed.

The only special case (apart from linear g) when the transformed model says anything useful about $\mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i\right]$ is the log transform. From

$$\log Y_i = \boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}_0 + \varepsilon_i$$

we get a multiplicative model

$$Y_i = \mathrm{e}^{\boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}_0}\varepsilon_i^*,$$

where $\varepsilon_i^* = \mathrm{e}^{\varepsilon_i}$, $\mathsf{E}\,\varepsilon_i^* = \mu_\varepsilon > 1$, $\mathsf{var}\,\varepsilon_i^* = \sigma_\varepsilon^2$. Then

$$\begin{aligned}\mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i\right] &= \exp\{\log\mu_\varepsilon + \boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}_0\},\\ \mathsf{var}\left[Y_i \middle| \boldsymbol{X}_i\right] &= \sigma_\varepsilon^2(\exp\{\boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}_0\})^2.\end{aligned}$$

While β_{01} (the intercept) does not have useful interpretation, the other parameters express multiplicative effects of $X_{i2},\ldots,X_{ip}$ on $\mathsf{E}\, Y_i$:

$$\mathrm{e}^{\beta_{0j}} = \frac{\mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i = \boldsymbol{x} + \boldsymbol{e}_j\right]}{\mathsf{E}\left[Y_i \middle| \boldsymbol{X}_i = \boldsymbol{x}\right]}, \quad j = 2,\ldots,p.$$

So, $\mathrm{e}^{\beta_{0j}}$ is the proportional increase (relative change) in $\mathsf{E}\, Y_i$ after a unit change in X_{ij}.

The problem with the interpretation of the transformed linear model is serious when the primary task is to estimate the effect of $\boldsymbol{X}_i$ on $\mathsf{E}\, Y_i$. If the goal is to predict Y_i from $\boldsymbol{X}_i$, transformations can still be useful even if the interpretation of the parameters is lost.

The end of lecture 1 (Mar. 1)

2. Generalized Linear Model: Theory

The generalized linear model extends the normal linear model in two aspects: it admits a wider choice of distributions for Y_i (distributions from the exponential family) and it allows some flexibility in the relationship between $\mathsf{E}\, Y_i$ and $\boldsymbol{X}_i^\top \boldsymbol{\beta}_0$.

2.1. Exponential Family

2.1.1. Parametrization, moments

Definition 2.1. A distribution of a real-valued random variable belongs to *the exponential family* of distributions[*] if its density (w.r.t. some σ-finite measure) can be written in the form

$$f(x;\theta,\varphi) = \exp\left\{\frac{x\theta - b(\theta)}{\varphi} + c(x,\varphi)\right\}, \tag{2.1}$$

where

- θ is called *the canonical parameter*[†];
- $\varphi \in (0,\infty)$ is called *the dispersion parameter*[‡];
- b and c are some real functions;

The expression (2.1) is called *the canonical form of the density*[§]. ∇

Example: Normal distribution

$Y \sim \mathsf{N}(\mu,\sigma^2)$, $\mu \in \mathbb{R}$, $\sigma^2 > 0$.

$$\begin{aligned} f(x;\mu,\sigma^2) &= \frac{1}{\sqrt{2\pi}\sigma}\exp\Big\{-\frac{(x-\mu)^2}{2\sigma^2}\Big\} \\ &= \frac{1}{\sqrt{2\pi}\sigma}\exp\Big\{\frac{x\mu}{\sigma^2} - \frac{\mu^2}{2\sigma^2} - \frac{x^2}{2\sigma^2}\Big\} \\ &= \exp\Big\{\frac{x\mu - \mu^2/2}{\sigma^2} - \frac{x^2}{2\sigma^2} - \frac{1}{2}\log(2\pi\sigma^2)\Big\}. \end{aligned}$$

[*] Česky *rozdělení exponenciálního typu* [†] Česky *kanonický parametr* [‡] Česky *disperzní parametr* [§] Česky *kanonický tvar hustoty*

$$\theta = \mu, \quad \varphi = \sigma^2, \quad b(\theta) = \frac{\theta^2}{2}, \quad c(x,\varphi) = -\frac{x^2}{2\varphi} - \frac{1}{2}\log(2\pi\varphi).$$

Example: Gamma distribution

$Y \sim \Gamma(a,p)$, $a > 0$, $p > 0$, $Y > 0$ a.s.

$$\begin{aligned} f(x;a,p) &= \frac{a^p}{\Gamma(p)} x^{p-1} \exp\{-ax\} \\ &= \exp\Big\{-ax + p\log a + (p-1)\log x - \log\Gamma(p)\Big\} \\ &= \exp\Big\{\frac{-(a/p)x + \log(a/p)}{1/p} + (p-1)\log x + p\log p - \log\Gamma(p)\Big\} \end{aligned}$$

$$\theta = -\frac{a}{p}, \quad \varphi = 1/p, \quad b(\theta) = -\log(-\theta)$$
$$c(x,\varphi) = (1/\varphi - 1)\log x - \log\varphi/\varphi - \log\Gamma(1/\varphi).$$

Example: Inverse Gaussian distribution

$Y \sim \mathsf{IG}(\mu,\lambda)$, $\mu > 0$, $\lambda > 0$, $Y > 0$ a.s.

$$\begin{aligned} f(x;\mu,\lambda) &= \sqrt{\frac{\lambda}{2\pi x^3}} \exp\Big\{-\frac{\lambda(x-\mu)^2}{2\mu^2 x}\Big\} \\ &= \sqrt{\frac{\lambda}{2\pi x^3}} \exp\Big\{-\frac{\lambda x^2}{2\mu^2 x} + \frac{\lambda x\mu}{\mu^2 x} - \frac{\lambda\mu^2}{2\mu^2 x}\Big\} \\ &= \exp\Big\{\frac{-x/(2\mu^2) + 1/\mu}{1/\lambda} + \frac{1}{2}\log\frac{\lambda}{2\pi x^3} - \frac{\lambda}{2x}\Big\}. \end{aligned}$$

$$\theta = -\frac{1}{2\mu^2}, \quad \varphi = 1/\lambda, \quad b(\theta) = -\sqrt{-2\theta}, \quad c(x,\varphi) = -\frac{1}{2}\log(2\pi x^3\varphi) - (2x\varphi)^{-1}.$$

This is a continuous distribution on the positive halfline. It is related to χ^2 distribution through the transformation

$$\frac{\lambda(X-\mu)^2}{\mu^2 X} \sim \chi^2_1.$$

Example: Poisson distribution

$Y \sim \mathsf{Po}(\lambda)$, $\lambda > 0$, values $0, 1, 2, \ldots$

$$f(x;\lambda) = \frac{\lambda^x}{x!}\exp\{-\lambda\} = \exp\bigl\{x\log\lambda - \lambda - \log x!\bigr\}.$$

$$\theta = \log\lambda, \quad \varphi = 1, \quad b(\theta) = \exp(\theta), \quad c(x,\varphi) = -\log x!$$

Example: Alternative distribution

$Y \sim \mathsf{Alt}(p)$, $p \in (0,1)$, values $0, 1$.

$$f(x;p) = p^x(1-p)^{1-x} = \exp\bigl\{x\log p + (1-x)\log(1-p)\bigr\} = \exp\Bigl\{x\log\frac{p}{1-p} + \log(1-p)\Bigr\}.$$

$$\theta = \log\frac{p}{1-p}, \quad \varphi = 1, \quad b(\theta) = \log(1+\mathrm{e}^\theta), \quad c(x,\varphi) = 0.$$

The next lemma shows that for distributions of exponential family, the first two moments can be obtained from the canonical form of the density by a simple calculation.

Lemma 2.1. *Let the random variable Y follow a distribution from the exponential family. Then the moment generation function $m_Y(t) \equiv \mathsf{E}\,\mathrm{e}^{tY}$ of Y exists, is finite, and is equal to*

$$m_Y(t) = \exp\left\{\frac{b(\theta+t\varphi) - b(\theta)}{\varphi}\right\}.$$

If $b(\theta)$ is twice continuously differentiable, $m_Y(t)$ is twice differentiable at $t = 0$, and

$$\begin{aligned} \mathsf{E}\,Y &= b'(\theta), \\ \mathsf{var}\,Y &= \varphi\, b''(\theta). \end{aligned}$$ ♢

Proof. Suppose the density $f(x;\theta,\varphi)$ exists with respect to a σ-finite measure ν and denote the support $A = \{x : f(x;\theta,\varphi) > 0\}$. We have

$$\begin{aligned} m_Y(t) = \mathsf{E}\,\mathrm{e}^{tY} &= \int_A \exp\left\{\frac{x\theta + xt\varphi - b(\theta)}{\varphi} + c(x,\varphi)\right\} d\nu(x) \\ &= \int_A \exp\left\{\frac{x(\theta+t\varphi) - b(\theta+t\varphi)}{\varphi} + c(x,\varphi)\right\} d\nu(x) \cdot \exp\left\{\frac{b(\theta+t\varphi) - b(\theta)}{\varphi}\right\} \\ &= \exp\left\{\frac{b(\theta+t\varphi) - b(\theta)}{\varphi}\right\}. \end{aligned}$$

The moments can be calculated by differentiation of $m_Y(t)$ at $t = 0$. We have $\mathsf{E}\, Y = m'_Y(0)$ and

$$m'_Y(t) = m_Y(t)\frac{b'(\theta + t\varphi)}{\varphi}\varphi,$$

so $\mathsf{E}\, Y = m'_Y(0) = b'(\theta)m_Y(0) = b'(\theta)$. Next, $\mathsf{E}\, Y^2 = m''_Y(0)$ and

$$m''_Y(t) = m_Y(t)\big[\, b'(\theta + t\varphi)\big]^2 + m_Y(t)b''(\theta + t\varphi)\varphi$$

so $\mathsf{E}\, Y^2 = m''_Y(0) = \varphi\, b''(\theta) + \big[\, b'(\theta)\big]^2$. Hence,

$$\mathsf{var}\, Y = \mathsf{E}\, Y^2 - \big(\mathsf{E}\, Y\big)^2 = \varphi\; b''(\theta). \qquad \square$$

We will always assume that $b(\theta)$ is twice continuously differentiable so that $\mathsf{var}\, Y$ is finite. Denote $\mu \overset{\text{df}}{=} \mathsf{E}\, Y$.

Note. Since $\mathsf{var}\, Y = \varphi\; b''(\theta) > 0$, b must be a strictly convex function and b' is strictly increasing. Hence b' has a well-defined inverse and there exists a function $V(\mu)$ of the mean μ such that $\mathsf{var}\, Y = \varphi V(\mu)$. It satisfies the equation $b''(\theta) = V(b'(\theta))$ or $V(\mu) = b''\big((b')^{-1}(\mu)\big)$.

Definition 2.2. The function $V(\mu)$ such that $\mathsf{var}\, Y = \varphi\, V(\mu)$ is called *the variance function**. ∇

Note.

- Different distributions that belong to the exponential family must have different variance functions.
- Within the exponential family, the variance function determines the distribution of Y. However, not every function V is a variance function of some distribution from the exponential family.

Example: Normal distribution

For $Y \sim \mathsf{N}(\mu, \sigma^2)$, we have $\theta = \mu$, $\varphi = \sigma^2$, and $b(\theta) = \frac{\theta^2}{2}$. Hence

$$\mathsf{E}\, Y = b'(\theta) = \mu, \quad \mathsf{var}\, Y = \varphi\; b''(\theta) = \varphi = \sigma^2, \quad \text{and} \quad V(\mu) = 1.$$

The normal distribution is the only distribution in exponential family with constant variance function, i.e., the variance is unrelated to the mean. (Recall the assumption of homoskedasticity in linear regression!).

* Česky *rozptylová funkce*

Example: Gamma distribution

For $Y \sim \Gamma(a,p)$, we have $\theta = -\frac{a}{p}$, $\varphi = 1/p$, and $b(\theta) = -\log(-\theta)$. Hence

$$\mu = \mathsf{E}\, Y = b'(\theta) = -1/\theta = p/a, \quad \mathsf{var}\, Y = \varphi\, b''(\theta) = \varphi/\theta^2 = p/a^2, \quad \text{and} \quad V(\mu) = \mu^2.$$

Example: Inverse Gaussian distribution

For $Y \sim \mathsf{IG}(\mu,\lambda)$, we have $\theta = -\frac{1}{2\mu^2}$, $\varphi = 1/\lambda$, and $b(\theta) = -\sqrt{-2\theta}$. Hence

$$\mathsf{E}\, Y = b'(\theta) = 1/\sqrt{-2\theta} = \mu, \quad \mathsf{var}\, Y = \varphi\, b''(\theta) = \varphi(-2\theta)^{-3/2} = \mu^3/\lambda, \quad \text{and} \quad V(\mu) = \mu^3.$$

Example: Poisson distribution

For $Y \sim \mathsf{Po}(\lambda)$, we have $\theta = \log\lambda$, $\varphi = 1$, and $b(\theta) = \exp(\theta)$. Hence

$$\mu = \mathsf{E}\, Y = b'(\theta) = \exp(\theta) = \lambda, \quad \mathsf{var}\, Y = \varphi\, b''(\theta) = \exp(\theta) = \lambda, \quad \text{and} \quad V(\mu) = \mu.$$

Example: Alternative distribution

For $Y \sim \mathsf{Alt}(p)$, we have $\theta = \log\frac{p}{1-p}$, $\varphi = 1$, and $b(\theta) = \log(1+\mathrm{e}^\theta) = \log(1-p)$. Hence

$$\mu = \mathsf{E}\, Y = b'(\theta) = \frac{\mathrm{e}^\theta}{1+\mathrm{e}^\theta} = p, \quad \mathsf{var}\, Y = \varphi\, b''(\theta) = \frac{\mathrm{e}^\theta}{(1+\mathrm{e}^\theta)^2} = p(1-p), V(\mu) = \mu(1-\mu).$$

2.1.2. Maximum likelihood estimator of the canonical parameter

Let $Y_1,\ldots,Y_n$ be a random sample from the density $f(x;\theta_0,\varphi_0)$ belonging to the exponential family, θ_0 is the true canonical parameter, φ_0 is the true dispersion parameter. Let $\boldsymbol{Y} = (Y_1,\ldots,Y_n)^\mathsf{T}$. We will discuss maximum likelihood estimation of the canonical parameter θ with iid data. Summary of the maximum likelihood theory together with notation we use throughout this text is provided in the Appendix starting on p. 62.

The likelihood for exponential family is

$$L(\theta,\varphi) = \prod_{i=1}^{n} \exp\left\{\frac{Y_i\theta - b(\theta)}{\varphi} + c(Y_i,\varphi)\right\},$$

The log-likelihood is

$$\ell(\theta,\varphi) = \log L(\theta,\varphi) = \sum_{i=1}^{n}\Big[\frac{Y_i\theta - b(\theta)}{\varphi} + c(Y_i,\varphi)\Big].$$

Suppose that the true dispersion parameter φ_0 is known. Then the score function for θ is

$$U(\theta \mid Y_i) = \frac{\partial}{\partial\theta}\log f(x;\theta,\varphi_0) = \frac{1}{\varphi_0}\big[Y_i - b'(\theta)\big].$$

Obviously, $\mathsf{E}\,U(\theta_0 \mid Y_i) = 0$. The score statistic is

$$U_n(\theta \mid \boldsymbol{Y}) = \sum_{i=1}^{n} U(\theta \mid Y_i) = \frac{1}{\varphi_0}\sum_{i=1}^{n}\big[Y_i - b'(\theta)\big].$$

The maximum likelihood estimator [MLE] $\widehat{\theta}_n$ solves the equation $U_n(\widehat{\theta}_n \mid \boldsymbol{Y}) = 0$, that is $\sum_{i=1}^{n} Y_i = nb'(\widehat{\theta}_n)$. The solution is $\widehat{\theta}_n = (b')^{-1}(\overline{Y}_n)$, where $\overline{Y}_n = n^{-1}\sum_{i=1}^{n} Y_i$.

The MLE is unique because b is convex, and it does not depend on the dispersion parameter φ_0. It can be calculated even if φ_0 is unknown.

The observed information is

$$I_n(\theta \mid \boldsymbol{Y}) = -\frac{1}{n}\sum_{i=1}^{n}\frac{\partial U(\theta \mid Y_i)}{\partial\theta} = \frac{1}{\varphi_0}b''(\theta) > 0,$$

so the likelihood is strictly concave. The expected (Fisher) information is the same as the observed information,

$$I(\theta) = -\mathsf{E}\,\frac{\partial U(\theta \mid Y_i)}{\partial\theta} = \frac{1}{\varphi_0}b''(\theta).$$

It is easy to check that

$$\mathsf{var}\,U(\theta_0 \mid Y_i) = I(\theta_0).$$

It follows from Theorem A.4 in the Appendix that

$$\sqrt{n}(\widehat{\theta}_n - \theta_0) \xrightarrow{\mathsf{D}} \mathsf{N}(0, \varphi_0[b''(\theta_0)]^{-1}). \tag{2.2}$$

Now consider the true dispersion parameter φ_0 unknown. The MLE of θ_0 is still the same, $\widehat{\theta}_n = (b')^{-1}(\overline{Y}_n)$. However, what is the asymptotic distribution of $\widehat{\theta}_n$ when φ_0 is unknown? In general, the asymptotic variance may change.

Calculate the joint information matrix for (θ,φ):

$$I(\theta_0,\varphi_0) = -\mathsf{E}\,\frac{\partial^2\log f(x;\theta_0,\varphi_0)}{\partial(\theta,\varphi)\partial(\theta,\varphi)^{\mathsf{T}}} = \begin{pmatrix} I_{\theta\theta} & I_{\theta\varphi} \\ I_{\theta\varphi} & I_{\varphi\varphi}\end{pmatrix} = \begin{pmatrix} b''(\theta_0)/\varphi_0 & 0 \\ 0 & I_{\varphi\varphi}\end{pmatrix}.$$

Thus, the information matrix is diagonal. It follows that the asymptotic distribution of $\widehat{\theta}_n$ is given by (2.2) even if φ_0 is unknown.

We do not need φ_0 to estimate θ_0 but we need an estimate of φ_0 to estimate the asymptotic variance of θ_0. Of course, we could use the MLE of φ_0 but it often cannot be calculated explicitely. Instead, we can use the moment estimator

$$\widehat{\varphi} = \frac{S_n^2}{b''(\widehat{\theta}_n)} = \frac{S_n^2}{V(\overline{Y}_n)},$$

where S_n^2 is the sample variance. Since $S_n^2 \xrightarrow{\mathsf{P}} \mathsf{var}\, Y_i = \varphi_0 b''(\theta_0)$, $\widehat{\theta}_n$ is consistent and b'' is continuous, $\widehat{\varphi}$ is consistent (though less efficient than the MLE).

The end of lecture 2 (Mar. 4)

2.2. Definition of the Generalized Linear Model

Consider n independent copies of random vectors $(Y_i, \boldsymbol{X}_i)$, $i = 1, \ldots, n$, where $\boldsymbol{X}_i = (X_{i1}, \ldots, X_{ip})^\mathsf{T}$. We want to express the dependence of $\mu_i \overset{\mathsf{df}}{=} \mathsf{E}\left[Y_i \,\middle|\, \boldsymbol{X}_i\right]$ on $\boldsymbol{X}_i$ by a model that is more general than the linear model.

Definition 2.3. (Nelder and Wedderburn 1972) The data $(Y_i, \boldsymbol{X}_i)$ satisfy the *generalized linear model** [GLM] if

1. $Y_1, \ldots, Y_n$ are independent and the distribution of Y_i depends on $\boldsymbol{X}_i$ through regression parameters $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)^\mathsf{T}$.
2. the conditional density of Y_i given $\boldsymbol{X}_i$ has the form

   $$f(y; \theta_i, \varphi) = \exp\left\{\frac{y\theta_i - b(\theta_i)}{\varphi} + c(y, \varphi)\right\},$$

   (is of exponential type), where $b(\cdot)$ is a known twice continuously differentiable function, θ_i depends on $\boldsymbol{X}_i$ and $\boldsymbol{\beta}$, $\varphi > 0$ is a known or an unknown constant.
3. θ_i depends on $\boldsymbol{X}_i$ and $\boldsymbol{\beta}$ through the *linear predictor*† $\eta_i \overset{\mathsf{df}}{=} \boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}$.
4. There exists a known strictly monotone, twice continuously differentiable *link function*‡ g such that $g(\mu_i) = \eta_i$. ∇

Notation. Let $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^\mathsf{T}$ and define the regression matrix

$$\mathbb{X}_{n\times p} = \begin{pmatrix} \boldsymbol{X}_1^\mathsf{T} \\ \boldsymbol{X}_2^\mathsf{T} \\ \vdots \\ \boldsymbol{X}_n^\mathsf{T} \end{pmatrix}.$$

We assume $r(\mathbb{X}) = p$. We sometimes use the notation $\boldsymbol{\beta}_0 = (\beta_{01}, \ldots, \beta_{0p})^\mathsf{T}$ to denote the true regression parameter (but the notation $\boldsymbol{\beta}$ can also mean the true parameter).

* Česky *zobecněný lineární model* † Česky *lineární prediktor* ‡ Česky *linková funkce*

Note. The (conditional) means of $Y_1, \ldots, Y_n$ vary because the canonical parameters $\theta_1, \ldots, \theta_n$ depend on $\boldsymbol{X}_i$. The dispersion parameter φ is the same for all observations, it must not depend on $\boldsymbol{X}_i$ (recall homoskedasticity in linear regression). However, the variances of $Y_1, \ldots, Y_n$ depend on the mean through the variance function $V(\mu_i)$, and hence vary with $\boldsymbol{X}_i$.

Note. The link function postulates a possibly non-linear relationship between the expectation of the response μ_i and the linear predictor $\eta_i = \boldsymbol{X}_i^\top \boldsymbol{\beta}$. It has to be specified in advance. There are methods to verify the choice of the link function for a specific data set (see Section 2.8.8). It is enough to specify the link function up to a non-zero proportionality constant (if $c \neq 0$, g and cg lead to the same model).

Definition 2.4. The link function g is called *the canonical link** for the distribution f if it equates the linear predictor η_i with the canonical parameter θ_i. ▽

Lemma 2.2. *(Properties of canonical link)*

(i) The canonical link is equal to the inverse of b', that is $g(\mu_i) = (b')^{-1}(\mu_i)$.
(ii) The canonical link satisfies the equation $g'(\mu_i) = 1/V(\mu_i)$. ◇

Proof. The link function g maps the mean $\mu_i = b'(\theta_i)$ to the linear predictor η_i: $g(\mu_i) = \eta_i$. The canonical link satisfies $\eta_i = \theta_i$.

For canonical link, $g(b'(\theta_i)) = \theta_i$, hence $g = (b')^{-1}$. This proves (i).

Differentiating the equality $g(b'(\theta_i)) = \theta_i$, we get $g'(b'(\theta_i))b''(\theta_i) = 1$. Because $b'(\theta_i) = \mu_i$ and $b''(\theta_i) = V(\mu_i)$, we get $g'(\mu_i)V(\mu_i) = 1$. This proves (ii). □

Note. For each distribution f from the exponential family, there is a unique (up to a non-zero proportionality constant) canonical link function. Two distributions cannot share the same canonical link. Canonical link functions have certain numerical advantages that will become apparent later on. However, some canonical link functions violate the conditions we require and are difficult to interpret (see examples below).

Example: Normal distribution

For normal distribution, the canonical parameter is $\theta_i = \mu_i$, and the dispersion parameter is $\varphi = \sigma^2$. Let $Y_i \sim \mathsf{N}(\mu_i, \sigma^2)$ with $g(\mu_i) = \boldsymbol{X}_i^\top \boldsymbol{\beta}$.

We know that

$$b(\theta_i) = \frac{\theta_i^2}{2}, \quad \mu_i = b'(\theta_i) = \theta_i, \quad \mathsf{var}\, Y_i = \sigma^2, \quad V(\mu) = 1.$$

* Česky *kanonický link*

The canonical link is $g(\mu_i) = (b')^{-1}(\mu_i) = \mu_i$ (identity link).

So the canonical GLM for the normal distribution is $\mathsf{E}\, Y_i = \eta_i = \boldsymbol{X}_i^\top \boldsymbol{\beta}$, the normal linear model.

Example: Gamma distribution

For gamma distribution, the canonical parameter is $\theta_i = -\frac{a_i}{p}$, and the dispersion parameter is $\varphi = 1/p$. So, we take $Y_i \sim \Gamma(a_i, p)$ with the mean $\mu_i = p/a_i$ and link $g(\mu_i) = \boldsymbol{X}_i^\top \boldsymbol{\beta}$.

We know that

$$b(\theta_i) = -\log(-\theta_i), \quad \mu_i = b'(\theta_i) = -1/\theta_i, \quad \mathsf{var}\, Y_i = \varphi \mu_i^2.$$

The canonical link is $g(\mu_i) = (b')^{-1}(\mu_i) \propto 1/\mu_i$ (inverse link — after dropping the minus sign). It is a function which is discontinuous at 0 and not strictly monotone.

The canonical GLM for the gamma distribution is $\mathsf{E}\, Y_i = g^{-1}(\eta_i) = 1/\boldsymbol{X}_i^\top \boldsymbol{\beta}$. The model can be interpreted only when the linear predictors have all either positive or negative signs.

Example: Inverse Gaussian distribution

For inverse Gaussian distribution, the canonical parameter is $\theta_i = -\frac{1}{2\mu_i^2}$, and the dispersion parameter is $\varphi = 1/\lambda$. So, we take $Y_i \sim \mathsf{IG}(\mu_i, \lambda)$ with the mean μ_i and link $g(\mu_i) = \boldsymbol{X}_i^\top \boldsymbol{\beta}$.

We know that

$$b(\theta_i) = -\sqrt{-2\theta_i}, \quad \mu_i = b'(\theta_i) = 1/\sqrt{-2\theta_i}, \quad \mathsf{var}\, Y_i = \varphi \mu_i^3.$$

The canonical link is $g(\mu_i) = (b')^{-1}(\mu_i) \propto 1/\mu_i^2$ (squared inverse link — after dropping the constant -2). It is a function which is discontinuous at 0 and not strictly monotone.

The canonical GLM for the inverse Gaussian distribution is $\mathsf{E}\, Y_i = g^{-1}(\eta_i) = 1/\sqrt{\boldsymbol{X}_i^\top \boldsymbol{\beta}}$. The model can be interpreted only when the linear predictors all have positive signs.

Example: Poisson distribution

For Poisson distribution, the canonical parameter is $\theta_i = \log \lambda_i$, and the dispersion parameter is $\varphi = 1$. So, we take $Y_i \sim \mathsf{Po}(\lambda_i)$ with the mean λ_i and link $g(\mu_i) = \boldsymbol{X}_i^\top \boldsymbol{\beta}$.

We know that

$$b(\theta_i) = \exp(\theta_i), \quad \mu_i = b'(\theta_i) = \exp(\theta_i), \quad \mathsf{var}\, Y_i = \mu_i.$$

The canonical link is $g(\mu_i) = (b')^{-1}(\mu_i) = \log \mu_i$ (log link).

The canonical GLM for Poisson distribution is $\mathsf{E}\, Y_i = g^{-1}(\eta_i) = \exp\{\boldsymbol{X}_i^\top \boldsymbol{\beta}\}$. This is called *the loglinear model*.

Example: Alternative distribution

For alternative distribution, the canonical parameter is $\theta_i = \log \frac{p_i}{1-p_i}$, and the dispersion parameter is $\varphi = 1$. So, we take $Y_i \sim \mathsf{Alt}(p_i)$ with the mean p_i and link $g(\mu_i) = \boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}$.
We know that

$$b(\theta_i) = \log(1 + \exp\{\theta_i\}), \quad \mu_i = b'(\theta_i) = \frac{\mathrm{e}^{\theta_i}}{1+\mathrm{e}^{\theta_i}}, \quad \mathsf{var}\, Y_i = \mu_i(1-\mu_i).$$

The canonical link is $g(\mu_i) = \log \frac{\mu_i}{1-\mu_i}$ (logistic link).

The canonical GLM for alternative distribution is $\mathsf{E}\, Y_i = g^{-1}(\eta_i) = \frac{\exp\{\boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}\}}{1+\exp\{\boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}\}}$. This is called *the logistic regression model*.

Choice of the link function

Canonical links provide very attractive options for the selection of the link function for normal, Poisson and alternative distributions. For these distributions, we always prefer the canonical link unless there is a very strong reason (given by the nature of the application) to select a different link function. For gamma and inverse Gaussian distributions, the canonical links are problematic because they do not even satisfy the assumptions we put on link functions. Also, they are hard to interpret.

Denote by $\mathscr{M}$ the parametric space for the mean of the response (the set of all possible values of the mean). Then g maps $\mathscr{M}$ to $\mathbb{R}$, which is the space of all possible values of the linear predictor. The inverse link g^{-1} should map $\mathbb{R}$ to $\mathscr{M}$.

For non-negative random variables, such as from gamma or inverse Gaussian distributions, $\mathscr{M} = (0, \infty)$. A reasonable inverse link g^{-1} should map $\mathbb{R}$ to $(0, \infty)$, but this is not the case for the canonical links of these two distributions. On the other hand, a reasonable link that maps the two sets correctly is the log-link. For this link, we get $\mu_i = \exp\{\boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}\}$, which is in $\mathscr{M}$ for any value of the parameter vector $\boldsymbol{\beta}$.

For the alternative distribution, $\mathscr{M} = (0, 1)$. A reasonable inverse link g^{-1} should map $\mathbb{R}$ to $(0, 1)$ and be strictly monotone. We can choose such links from distribution functions of continuous random variables with positive densities over $\mathbb{R}$. On the other hand, the link functions are quantile functions of such distributions. The logistic link is the quantile function of the standard logistic distribution.

Parametrizations of the GLM

The primary parameters in the GLM are the regression coefficients $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)^\mathsf{T}$. However, we are also interested in parametrizing the distributions of the individual Y_i's that

depend on both the primary parameters $\boldsymbol{\beta}$ and the covariates $\boldsymbol{X}_i$. This can be done in three ways:

- by the *linear predictors* $\eta_1, \ldots, \eta_n$;
- by the *means* $\mu_1 \equiv \mathsf{E}\, Y_1, \ldots, \mu_n \equiv \mathsf{E}\, Y_n$;
- by the *canonical parameters* $\theta_1, \ldots, \theta_n$.

The parametrizations are related to each other as follows:

- $\eta_i = \boldsymbol{X}_i^\top \boldsymbol{\beta}$;
- $\eta_i = g(\mu_i)$, $\mu_i = g^{-1}(\eta_i)$;
- $\mu_i = b'(\theta_i)$, $\theta_i = (b')^{-1}(\mu_i)$;
- $\eta_i = g\big(b'(\theta_i)\big)$, $\theta_i = (b')^{-1}\big(g^{-1}(\eta_i)\big)$; if the link g is canonical then $\eta_i = \theta_i$.

The end of lecture 3 (Mar. 4)

The likelihood function

Let the true dispersion parameter φ_0 be known. The likelihood function for $\boldsymbol{\beta}$ has the form

$$L(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \prod_{i=1}^{n} \exp\left\{ \frac{Y_i \theta_i - b(\theta_i)}{\varphi_0} + c(Y_i, \varphi_0) \right\},$$

where $\theta_i = (b')^{-1}\big(g^{-1}(\boldsymbol{X}_i^\top \boldsymbol{\beta})\big)$.

The log-likelihood is

$$\ell(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \sum_{i=1}^{n} \left[\frac{Y_i \theta_i - b(\theta_i)}{\varphi_0} + c(Y_i, \varphi_0) \right]. \tag{2.3}$$

The saturated model

Suppose at least one covariate is continuous and consider a model which has the largest possible number of parameters $p = n$. This is called *the saturated model*[*]. In the saturated model, each Y_i gets its own canonical parameter θ_i, which is unrelated to the canonical parameters of the other observations. Maximizing $L(\boldsymbol{\beta} \mid \boldsymbol{Y})$ w.r.t all $\boldsymbol{\beta} \in \mathbb{R}^n$ is the same as maximizing $L(\boldsymbol{\theta} \mid \boldsymbol{Y})$ w.r.t all $\boldsymbol{\theta} \in \mathbb{R}^n$. To obtain the MLE in the saturated model, we differentiate (2.3) w.r.t. each θ_i separately and we get n equations

$$\varphi_0^{-1}[Y_i - b'(\theta_i)] = 0, \quad i = 1, \ldots, n.$$

The MLE of μ_i under the saturated model is

$$\widehat{\mu}_i = Y_i.$$

[*] Česky *saturovaný model*

The fitted values $\widehat{\mu}_i \equiv \widehat{Y}_i$ are equal to the observed values Y_i. This model provides a "perfect fit". However, a "perfect fit" of this kind is rarely useful.

The saturated model with $p = n$ does not satisfy the regularity assumptions of the MLE theory (the number of parameters must be constant for the theory to apply; here $p \to \infty$ as $n \to \infty$). The estimates obtained from this model are not even consistent.

Note. When all covariates are discrete (with a finite number of values), the largest possible number of parameters in the model is equal to the number of possible distinct values of the covariate vector $\boldsymbol{X}_i$, which is usually smaller than n and does not change as the number of observations increases. In this setting, the saturated model behaves differently.

The null model

The null model[*] is the opposite extreme. It assumes $p = 1$ and $\boldsymbol{X}_i = 1$ so that the model includes only the intercept and all Y_i are equally distributed.

The MLE of the common canonical parameter θ of the null model is derived in Section 2.1.2. Using $\beta_0 = \eta = g\big(b'(\theta)\big)$, we get the MLE of β_0 as $\widehat{\beta}_n = g(b'(\widehat{\theta}_n)) = g(\overline{Y}_n)$. From the central limit theorem for iid random variables and the delta method,

$$\sqrt{n}(\widehat{\beta}_n - \beta_0) \xrightarrow{\mathsf{D}} \mathsf{N}(0, \varphi_0 V(\mu_0)[g'(\mu_0)]^2),$$

where $\mu_0 = \mathsf{E}\, Y_i$ (compare this with (2.2)).

Neither the null model nor the saturated model are particularly interesting. We aim to build a model which has more structure than the null model, fewer parameters than the saturated model, and fits the observed data well.

2.3. Maximum Likelihood Estimation in the GLM

Let $(Y_i, \boldsymbol{X}_i)$, $i = 1, \ldots, n$ be iid random vectors of dimension $p+1$. Let $h_i(\boldsymbol{x})$ be the marginal density of $\boldsymbol{X}_i$ (with no assumptions about it except finite second moments). Let $(Y_i, \boldsymbol{X}_i)$, $i = 1, \ldots, n$, satisfy the generalized linear model (Definition 2.3) with true parameters $\boldsymbol{\beta}_0$ and φ_0. Consider φ_0 known. Write the conditional density of Y given $\boldsymbol{X} = \boldsymbol{x}$ as $f(y \mid \boldsymbol{x}, \boldsymbol{\beta}_0, \varphi_0)$. Then the joint density of $(Y_i, \boldsymbol{X}_i)$ is $f(y \mid \boldsymbol{x}, \boldsymbol{\beta}_0, \varphi_0) h_i(\boldsymbol{x})$, the full likelihood is

$$L^*(\boldsymbol{\beta}) = \prod_{i=1}^{n} f(Y_i \mid \boldsymbol{X}_i, \boldsymbol{\beta}, \varphi_0)\, h_i(\boldsymbol{X}_i)$$

and the full log-likelihood is

$$\ell^*(\boldsymbol{\beta}) = \sum_{i=1}^{n} \log f(Y_i \mid \boldsymbol{X}_i, \boldsymbol{\beta}, \varphi_0) + \sum_{i=1}^{n} \log h_i(\boldsymbol{X}_i).$$

[*] Česky *nulový model*

Since the rightmost sum does not depend on $\boldsymbol{\beta}$, it suffices to maximize

$$\ell(\boldsymbol{\beta}) = \sum_{i=1}^{n} \log f(Y_i \mid \boldsymbol{X}_i, \boldsymbol{\beta}, \varphi_0). \tag{2.4}$$

This is the log-likelihood shown previously in (2.3) (without the detailed derivation and justification needed for the validity of asymptotic results).

When the covariates are random, it is not necessary to consider, know or estimate their distribution. If the covariates were constants, the log-likelihood and the score statistic would be sums of nonidentically distributed terms. Feller-Lindeberg or Lyapunov central limit theorems would have to be applied to validate the asymptotic results, and additional assumptions would have to be imposed on the covariates. The asymptotic results for constant covariates would then turn out to be the same as the results for iid data.

The core term in the log-likelihood (2.4) that we are going to maximize can be written as

$$\sum_{i=1}^{n} \frac{Y_i\theta_i - b(\theta_i)}{\varphi_0}, \tag{2.5}$$

where $g(\mu_i) = \boldsymbol{X}_i^{\mathsf{T}}\boldsymbol{\beta}$ and $\mu_i = b'(\theta_i)$. The following theorem summarizes the main results for maximum likelihood estimation of $\boldsymbol{\beta}$.

Theorem 2.3. *(likelihood equations in the GLM; Nelder and Wedderburn 1972) Let the definition of the GLM hold. Denote by $\boldsymbol{\beta}_0$ the true parameter. Let*

$$w(\mu_i) = \frac{1}{V(\mu_i)[g'(\mu_i)]^2} > 0. \tag{2.6}$$

(i) The score function for $\boldsymbol{\beta}$ is

$$\boldsymbol{U}(\boldsymbol{\beta} \mid Y_i) = \varphi_0^{-1} w(\mu_i) g'(\mu_i)(Y_i - \mu_i)\boldsymbol{X}_i,$$

where $\mu_i = g^{-1}(\boldsymbol{X}_i^T\boldsymbol{\beta})$. It satisfies $E\,\boldsymbol{U}(\boldsymbol{\beta}_0 \mid Y_i) = \boldsymbol{0}$.

(ii) The score statistic for $\boldsymbol{\beta}$ is

$$\boldsymbol{U}_n(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \frac{1}{\varphi_0} \sum_{i=1}^{n} w(\mu_i) g'(\mu_i)(Y_i - \mu_i)\boldsymbol{X}_i.$$

(iii) The maximum likelihood estimator $\widehat{\boldsymbol{\beta}}_n$ solves the system of equations

$$\sum_{i=1}^{n} w(\widehat{\mu}_i) g'(\widehat{\mu}_i)(Y_i - \widehat{\mu}_i)\boldsymbol{X}_i = \boldsymbol{0}, \tag{2.7}$$

where $\widehat{\mu}_i = g^{-1}(\boldsymbol{X}_i^T\widehat{\boldsymbol{\beta}}_n)$.

(iv) *When the link g is canonical then*

$$w(\mu_i) = V(\mu_i) = \frac{1}{g'(\mu_i)},$$

the score statistic can be written as

$$\boldsymbol{U}_n(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \frac{1}{\varphi_0} \sum_{i=1}^{n} (Y_i - \mu_i)\boldsymbol{X}_i,$$

and the likelihood equations are

$$\sum_{i=1}^{n} Y_i \boldsymbol{X}_i = \sum_{i=1}^{n} \widehat{\mu}_i \boldsymbol{X}_i.$$

♢

Note. When the link g is canonical then $\boldsymbol{S} = \sum_{i=1}^{n} Y_i \boldsymbol{X}_i$ is the sufficient statistic and the MLE equates the observed value of $\boldsymbol{S}$ to its estimated expectation under the model (conditional on the covariates).

Definition 2.5. $\widehat{\mu}_i = g^{-1}(\boldsymbol{X}_i^\top \widehat{\boldsymbol{\beta}}_n)$ are called *the fitted values**. ▽

Proof (of Theorem 2.3).

(i) The score function is calculated by the chain rule:

$$\boldsymbol{U}(\boldsymbol{\beta} \mid Y_i) = \frac{\partial}{\partial \boldsymbol{\beta}} \frac{1}{\varphi_0}[Y_i\theta_i - b(\theta_i)] = \frac{\partial}{\partial \theta} \frac{1}{\varphi_0}[Y_i\theta_i - b(\theta_i)] \cdot \frac{\partial \theta_i}{\partial \mu} \cdot \frac{\partial \mu_i}{\partial \eta} \cdot \frac{\partial \eta_i}{\partial \boldsymbol{\beta}}$$

This is a product of four terms. The first term is $\frac{1}{\varphi_0}(Y_i - \mu_i)$. The next two terms can be calculated by the formula for the derivative of the inverse function. We have

$$\frac{\partial \theta_i}{\partial \mu} = \frac{\partial (b')^{-1}(\mu_i)}{\partial \mu} = \frac{1}{b''(\theta_i)} = \frac{1}{V(\mu_i)},$$

and

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

Finally, $\frac{\partial \eta_i}{\partial \boldsymbol{\beta}} = \frac{\partial \boldsymbol{X}_i^\top \boldsymbol{\beta}}{\partial \boldsymbol{\beta}} = \boldsymbol{X}_i$. So we have

$$\boldsymbol{U}(\boldsymbol{\beta} \mid Y_i) = \frac{Y_i - \mu_i}{\varphi_0 V(\mu_i) g'(\mu_i)} \boldsymbol{X}_i = \frac{1}{\varphi_0} \underbrace{\frac{1}{V(\mu_i)[g'(\mu_i)]^2}}_{\stackrel{\text{df}}{=} w(\mu_i) > 0} g'(\mu_i)(Y_i - \mu_i)\boldsymbol{X}_i.$$

* Česky *vyrovnané hodnoty*

Because the conditional expectation (given $\boldsymbol{X}_i$) of $Y_i - \mu_i$ is 0 when μ_i is evaluated at the true parameter $\boldsymbol{\beta}_0$, the conditional expectation of $\boldsymbol{U}(\boldsymbol{\beta}_0 \mid Y_i)$ is zero and the unconditional expectation is zero as well. This proves that $\mathsf{E}\,\boldsymbol{U}(\boldsymbol{\beta}_0 \mid Y_i) = \boldsymbol{0}$.

The next two points (ii) and (iii) are obvious.

(iv) For the canonical link, we know by Lemma 2.2 that $g'(\mu_i) = 1/V(\mu_i)$. Hence $w(\mu_i) = V(\mu_i)$ and $w(\mu_i)g'(\mu_i) = 1$. The rest is easy. □

The end of lecture 4 (Mar. 11)

The next step is to investigate the observed and expected information matrices for $\boldsymbol{\beta}$. Let $\boldsymbol{a}^{\otimes 2} \stackrel{\mathrm{df}}{=} \boldsymbol{a}\boldsymbol{a}^{\mathsf{T}}$.

Theorem 2.4. *(on information matrices in the GLM) Let the definition of the GLM hold. Let $\mathsf{E}_{\boldsymbol{X}} w(\mu_i)\boldsymbol{X}_i^{\otimes 2}$ be finite and of full rank.*

(i) The contribution of the i-th observation to the observed information matrix is

$$I(\boldsymbol{\beta} \mid Y_i) = \frac{1}{\varphi_0}\big[w(\mu_i)\boldsymbol{X}_i^{\otimes 2} - \mathbb{J}_i\big],$$

where

$$\mathbb{J}_i = \left[w'(\mu_i) + w(\mu_i)\frac{g''(\mu_i)}{g'(\mu_i)}\right](Y_i - \mu_i)\boldsymbol{X}_i^{\otimes 2}.$$

The observed information matrix is $I_n(\boldsymbol{\beta} \mid \boldsymbol{Y}) = n^{-1}\sum_{i=1}^n I(\boldsymbol{\beta} \mid Y_i)$.

(ii) When evaluated at the true $\boldsymbol{\beta}_0$, $\mathsf{E}\,\mathbb{J}_i = 0$. The Fisher (expected) information matrix at the true $\boldsymbol{\beta}_0$ is

$$I(\boldsymbol{\beta}_0) = \mathsf{E}\, I(\boldsymbol{\beta}_0 \mid Y_i) = \frac{1}{\varphi_0}\mathsf{E}_{\boldsymbol{X}} w(\mu_i)\boldsymbol{X}_i^{\otimes 2}. \tag{2.8}$$

By assumptions, it is finite and of full rank. It holds that $\mathrm{var}\,\boldsymbol{U}(\boldsymbol{\beta}_0 \mid Y_i) = I(\boldsymbol{\beta}_0)$.

(iii) When the link g is canonical then $\mathbb{J}_i = 0$ at any $\boldsymbol{\beta}$ for all i, the observed information matrix is positive definite at all $\boldsymbol{\beta}$, the log-likelihood is concave, the likelihood equations have just one solution and it is the MLE. ♢

Note. If the link g is not canonical, there is no guarantee that a solution to the likelihood equations is the MLE. The likelihood is not concave, the equations may have multiple solutions. Numerical algorithms for solving the likelihood equations may iterate slowly and converge to the wrong solution.

The Fisher information matrix $I(\boldsymbol{\beta}_0)$ can be consistently estimated by the empirical estimator

$$\widehat{I}_n = \frac{1}{n\varphi_0}\sum_{i=1}^n w(\widehat{\mu}_i)\boldsymbol{X}_i^{\otimes 2} = \frac{1}{n\varphi_0}\mathbb{X}^{\mathsf{T}}\hat{\mathbb{W}}\mathbb{X}, \tag{2.9}$$

where $\hat{\mathbb{W}}$ is the $n \times n$ diagonal matrix $\mathrm{diag}\,(w(\widehat{\mu}_1), \ldots, w(\widehat{\mu}_n))$. When φ_0 is unknown it is replaced by a consistent estimator $\widehat{\varphi}_n$, which will be introduced in Section 2.5.

Proof (of Theorem 2.4).

(i) The contribution to the observed information matrix can be calculated as follows.

$$I(\boldsymbol{\beta} \mid Y_i) = -\frac{\partial}{\partial \boldsymbol{\beta}^\top} \boldsymbol{U}(\boldsymbol{\beta} \mid Y_i) = -\frac{1}{\varphi_0} \frac{\partial w(\mu_i) g'(\mu_i)(Y_i - \mu_i)}{\partial \mu} \boldsymbol{X}_i \cdot \frac{\partial \mu_i}{\partial \eta} \cdot \frac{\partial \eta_i}{\partial \boldsymbol{\beta}^\top}.$$

We already know from the proof of Theorem 2.3 that

$$\frac{\partial \mu_i}{\partial \eta} = \frac{1}{g'(\mu_i)} \quad \text{and} \quad \frac{\partial \eta_i}{\partial \boldsymbol{\beta}^\top} = \boldsymbol{X}_i^\top.$$

It remains to calculate the derivative of the product of three functions of μ_i. We get

$$\frac{\partial w(\mu_i) g'(\mu_i)(Y_i - \mu_i)}{\partial \mu} = w'(\mu_i) g'(\mu_i)(Y_i - \mu_i) + w(\mu_i) g''(\mu_i)(Y_i - \mu_i) - w(\mu_i) g'(\mu_i).$$

Putting all the terms together and separating out the part that does not depend on $(Y_i - \mu_i)$, we get

$$I(\boldsymbol{\beta} \mid Y_i) = \frac{1}{\varphi_0} w(\mu_i) \boldsymbol{X}_i \boldsymbol{X}_i^\top - \frac{1}{\varphi_0} \underbrace{\left[w'(\mu_i) + w(\mu_i) \frac{g''(\mu_i)}{g'(\mu_i)} \right]}_{\stackrel{\text{df}}{=} \mathbb{J}_i} (Y_i - \mu_i) \boldsymbol{X}_i \boldsymbol{X}_i^\top$$

and the result follows. Notice that the first part is a positive semi-definite matrix while the second part may be anything.

(ii) Because $\mathbb{J}_i$ is a product of $Y_i - \mu_i$ (which has zero conditional expectation given $\boldsymbol{X}_i$ at the true $\boldsymbol{\beta}_0$) and terms that depend on $\boldsymbol{X}_i$ but not on Y_i, its expectation at the true $\boldsymbol{\beta}_0$ is a zero matrix. It follows that

$$\mathsf{E}\, I(\boldsymbol{\beta}_0 \mid Y_i) = \frac{1}{\varphi_0} \mathsf{E}_X w(\mu_i) \boldsymbol{X}_i^{\otimes 2}.$$

Next,

$$\begin{aligned} \mathsf{var}\, \boldsymbol{U}(\boldsymbol{\beta}_0 \mid Y_i) &= \mathsf{var}\, \frac{1}{\varphi_0} w(\mu_i) g'(\mu_i)(Y_i - \mu_i) \boldsymbol{X}_i = \mathsf{E}_X \frac{1}{\varphi_0^2} [w(\mu_i) g'(\mu_i)]^2 \mathsf{var}\left[Y_i \,\middle|\, \boldsymbol{X}_i \right] \boldsymbol{X}_i^{\otimes 2} \\ &= \mathsf{E}_X \frac{[w(\mu_i) g'(\mu_i)]^2 \varphi_0 V(\mu_i)}{\varphi_0^2} \boldsymbol{X}_i^{\otimes 2} = \frac{1}{\varphi_0} \mathsf{E}_X w(\mu_i) \boldsymbol{X}_i^{\otimes 2} = I(\boldsymbol{\beta}_0 \mid Y_i). \end{aligned}$$

(iii) We have $w(\mu_i) = \frac{1}{V(\mu_i)[g'(\mu_i)]^2}$. For the canonical link, $g'(\mu_i) = 1/V(\mu_i)$ by Lemma 2.2, hence $g'(\mu_i) = 1/w(\mu_i)$. Next,

$$g''(\mu_i) = -\frac{w'(\mu_i)}{w^2(\mu_i)}.$$

Hence

$$\frac{g''(\mu_i)}{g'(\mu_i)} w(\mu_i) = -w'(\mu_i) \quad \text{and} \quad \left[w'(\mu_i) + w(\mu_i) \frac{g''(\mu_i)}{g'(\mu_i)} \right] = 0. \qquad \square$$

2.4. Algorithm for Fitting the GLM

The parameters of the GLM can be estimated by a numerical algorithm called *iterative weighted least squares*[*] [IWLS]. It is based on the following result.

Theorem 2.5. *(Nelder and Wedderburn 1972) The MLE $\widehat{\boldsymbol{\beta}}_n$ in the GLM solves the system of equations*

$$\widehat{\boldsymbol{\beta}}_n = (\mathbb{X}^T\hat{\mathbb{W}}\mathbb{X})^{-1}(\mathbb{X}^T\hat{\mathbb{W}}\widehat{\boldsymbol{Z}}),$$

where $\hat{\mathbb{W}} = \operatorname{diag}(w(\widehat{\mu}_1),\dots,w(\widehat{\mu}_n))$, $\widehat{\boldsymbol{Z}}$ is an n-vector with components

$$\widehat{Z}_i = \widehat{\eta}_i + (Y_i - \widehat{\mu}_i)g'(\widehat{\mu}_i),$$

$\widehat{\mu}_i = g^{-1}(\widehat{\eta}_i)$, and $\widehat{\eta}_i = \boldsymbol{X}_i^T\widehat{\boldsymbol{\beta}}_n$. ♢

Note. $\widehat{\boldsymbol{Z}}$ is called *the adjusted dependent variable*[†]. Notice that $\widehat{Z}_i$ is the linear approximation to $g(Y_i)$ by Taylor expansion around $\widehat{\mu}_i$:

$$g(Y_i) \approx g(\widehat{\mu}_i) + g'(\widehat{\mu}_i)(Y_i - \widehat{\mu}_i).$$

Unlike $g(Y_i)$, the adjusted dependent variable can be calculated even if Y_i is outside of the domain of g, for example when $g \equiv \log$ and $Y_i \sim \mathsf{Po}(\mu_i)$ attains the value of zero.

Note. When the link g is canonical then $\hat{\mathbb{W}} = \operatorname{diag}(V(\widehat{\mu}_1),\dots,V(\widehat{\mu}_n))$ and

$$\widehat{Z}_i = \widehat{\eta}_i + \frac{Y_i - \widehat{\mu}_i}{V(\widehat{\mu}_i)}.$$

Proof (of Theorem 2.5). Take the obvious equality

$$\left(\sum_{i=1}^n w(\widehat{\mu}_i)\boldsymbol{X}_i\boldsymbol{X}_i^\mathsf{T}\right)\widehat{\boldsymbol{\beta}}_n = \left(\sum_{i=1}^n w(\widehat{\mu}_i)\boldsymbol{X}_i\boldsymbol{X}_i^\mathsf{T}\right)\widehat{\boldsymbol{\beta}}_n$$

and add zero to the right-hand side in the form of the likelihood equations

$$\mathbf{0} = \sum_{i=1}^n w(\widehat{\mu}_i)g'(\widehat{\mu}_i)(Y_i - \widehat{\mu}_i)\boldsymbol{X}_i.$$

Rearrange the right-hand side to get

$$\left(\sum_{i=1}^n w(\widehat{\mu}_i)\boldsymbol{X}_i\boldsymbol{X}_i^\mathsf{T}\right)\widehat{\boldsymbol{\beta}}_n = \sum_{i=1}^n w(\widehat{\mu}_i)\boldsymbol{X}_i\left[\boldsymbol{X}_i^\mathsf{T}\widehat{\boldsymbol{\beta}}_n + g'(\widehat{\mu}_i)(Y_i - \widehat{\mu}_i)\right],$$

where the bracket contains the value $\widehat{Z}_i$ of the adjusted dependent variable. Rewrite the result in a matrix form as

$$(\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}\mathbb{X})\widehat{\boldsymbol{\beta}}_n = \mathbb{X}^\mathsf{T}\hat{\mathbb{W}}\widehat{\boldsymbol{Z}}.$$

This completes the proof. □

[*] Česky *iterativní vážené nejmenší čtverce* [†] Česky *upravená odezva*

One cannot calculate $\widehat{\boldsymbol{\beta}}_n$ directly from Theorem 2.5 because it appears on both the left-hand side as well as the right-hand side. However, the result motivates the following iterative algorithm.

Iterative weighted least squares algorithm

Step 1. Take initial values $\widehat{\mu}_i^{(0)} = Y_i$ (or $Y_i \pm \varepsilon$ if Y_i is not within the domain of g). Set $k := 0$.

Step 2. Calculate $\hat{\mathbb{W}}^{(k)} = \mathrm{diag}\,(w(\widehat{\mu}_1^{(k)}), \ldots, w(\widehat{\mu}_n^{(k)}))$ and $\widehat{Z}_i^{(k)} = g(\widehat{\mu}_i^{(k)}) + (Y_i - \widehat{\mu}_i^{(k)}) g'(\widehat{\mu}_i^{(k)})$.

Step 3. Take

$$\widehat{\boldsymbol{\beta}}_n^{(k+1)} = (\mathbb{X}^\mathsf{T} \hat{\mathbb{W}}^{(k)} \mathbb{X})^{-1} (\mathbb{X}^\mathsf{T} \hat{\mathbb{W}}^{(k)} \widehat{\boldsymbol{Z}}^{(k)}).$$

Step 4. Calculate $\widehat{\mu}_i^{(k+1)} = g^{-1}(\boldsymbol{X}_i^\mathsf{T} \widehat{\boldsymbol{\beta}}_n^{(k+1)})$.

Step 5. Set $k := k + 1$.

Iterate steps 2–5 until convergence, for example until $\left\| \widehat{\boldsymbol{\beta}}_n^{(k)} - \widehat{\boldsymbol{\beta}}_n^{(k-1)} \right\| < \delta$, where δ is a pre-specified tolerance parameter. If the model is well formulated, the algorithm usually converges in 5–7 steps.

Note.

- The IWLS algorithm is a special case of the Fisher scoring algorithm (see Appendix A.2, bottom of page 64).
- According to (2.9), the matrix $(\mathbb{X}^\mathsf{T} \hat{\mathbb{W}}^{(k)} \mathbb{X})^{-1}$ estimates (up to the proportionality constant φ_0) the inverse information matrix. Thus, an estimate of the asymptotic variance of $\widehat{\boldsymbol{\beta}}_n$ is obtained by the IWLS as well (just make sure to update it after the last iteration of $\widehat{\boldsymbol{\beta}}_n^{(k)}$).
- Let $\mathbb{X}^* = \hat{\mathbb{W}}^{1/2} \mathbb{X}$ and $\boldsymbol{Y}^* = \hat{\mathbb{W}}^{1/2} \widehat{\boldsymbol{Z}}$. Then $\widehat{\boldsymbol{\beta}}_n$ can be written as an ordinary least squares estimator $\widehat{\boldsymbol{\beta}}_n = (\mathbb{X}^{*\mathsf{T}} \mathbb{X}^*)^{-1} \mathbb{X}^{*\mathsf{T}} \boldsymbol{Y}^*$. This is useful for extending the diagnostic methods available for the linear model to the GLM.

The end of lecture 5 (Mar. 11)

2.5. Estimation of the Dispersion Parameter

The dispersion parameter φ_0 is usually unknown (unless we work with Poisson or alternative distributions). This fact does not alter the estimation of $\boldsymbol{\beta}_0$ or the asymptotic properties of $\widehat{\boldsymbol{\beta}}_n$ but we occassionally need an estimator for φ_0. Instead of using the method of maximum likelihood, φ_0 is estimated by a modified method of moments.

Definition 2.6. The statistic

$$X^2 = \sum_{i=1}^{n} \frac{(Y_i - \widehat{\mu}_i)^2}{V(\widehat{\mu}_i)} \tag{2.10}$$

is called *the Pearson chi-square statistic*[*]. An estimator for φ_0 is given by

$$\widehat{\varphi}_n = \frac{X^2}{n-p}. \tag{2.11}$$

▽

Note. When the distribution of Y_i is normal, X^2 is the residual sum of squares SS_e and $\widehat{\varphi}_n$ is the usual estimator of residual variance.

The next theorem provides conditions for consistency of $\widehat{\varphi}_n$.

Theorem 2.6. *Let $h(y, \boldsymbol{x}, \boldsymbol{\beta}) = \frac{[y - g^{-1}(\boldsymbol{x}^T\boldsymbol{\beta})]^2}{V(g^{-1}(\boldsymbol{x}^T\boldsymbol{\beta}))}$. Suppose there exists a function $C(y, \boldsymbol{x})$ such that $\|\partial h/\partial \boldsymbol{\beta}\| \le C(y, \boldsymbol{x})$ in a neighborhood $\mathcal{B}_0$ of $\boldsymbol{\beta}_0$ and $\mathsf{E}\, C(Y_i, \boldsymbol{X}_i)$ exists and is finite. Then $\widehat{\varphi}_n \xrightarrow{P} \varphi_0$.* ◇

Note. The notation $\|\cdot\|$ means the Euclidean norm. The condition of Theorem 2.6 is fulfilled when V and g' are bounded away from zero and V has a bounded derivative in a neighborhood of $\boldsymbol{\beta}_0$.

Note. The moment estimator $\widehat{\varphi}_n$ is used instead of φ_0 in all statistics that need to be evaluated. The asymptotic distributions of these statistics are not affected (Cramér-Slutski Theorem).

Proof. We have

$$\widehat{\varphi}_n = \frac{1}{n-p} \sum_{i=1}^{n} h(Y_i, \boldsymbol{X}_i, \widehat{\boldsymbol{\beta}}_n).$$

Decompose this as follows:

$$\widehat{\varphi}_n = \frac{1}{n-p} \sum_{i=1}^{n} h(Y_i, \boldsymbol{X}_i, \boldsymbol{\beta}_0) + \frac{1}{n-p} \sum_{i=1}^{n} [h(Y_i, \boldsymbol{X}_i, \widehat{\boldsymbol{\beta}}_n) - h(Y_i, \boldsymbol{X}_i, \boldsymbol{\beta}_0)].$$

The first summand is an average of iid terms that converges in probability by the weak law of large numbers to

$$\mathsf{E}\, h(Y_i, \boldsymbol{X}_i, \boldsymbol{\beta}_0) = \mathsf{E}\, \mathsf{E}\Big[\frac{(Y_i - \mu_i)^2}{V(\mu_i)} \,\Big|\, \boldsymbol{X}_i\Big] = \mathsf{E}\, \frac{\varphi_0 V(\mu_i)}{V(\mu_i)} = \varphi_0.$$

We need to prove that the second summand converges in probability to 0. Take its Euclidean norm, ignore the subtraction of p from n in the denominator, and bound it from above using a one-step Taylor expansion

$$\left\| \frac{1}{n} \sum_{i=1}^{n} [h(Y_i, \boldsymbol{X}_i, \widehat{\boldsymbol{\beta}}_n) - h(Y_i, \boldsymbol{X}_i, \boldsymbol{\beta}_0)] \right\| \le \left\| \widehat{\boldsymbol{\beta}}_n - \boldsymbol{\beta}_0 \right\| \frac{1}{n} \sum_{i=1}^{n} \left\| h'(Y_i, \boldsymbol{X}_i, \boldsymbol{\beta}^*) \right\|,$$

[*] Česky *Pearsonovo chí kvadrát*

where $\boldsymbol{\beta}^*$ lies on the line segment between $\widehat{\boldsymbol{\beta}}_n$ and $\boldsymbol{\beta}_0$, and $h'(y, \boldsymbol{x}, \beta) = \partial h / \partial \boldsymbol{\beta}$. The estimator $\widehat{\boldsymbol{\beta}}_n$ is consistent, so $\left\| \widehat{\boldsymbol{\beta}}_n - \boldsymbol{\beta}_0 \right\| \xrightarrow{\mathsf{P}} 0$ and $\|\boldsymbol{\beta}^* - \boldsymbol{\beta}_0\| \xrightarrow{\mathsf{P}} 0$.

It remains to show that $\frac{1}{n}\sum_{i=1}^{n} \left\| h'(Y_i, \boldsymbol{X}_i, \boldsymbol{\beta}^*) \right\|$ is bounded from above in probability by a constant. Since $\boldsymbol{\beta}^*$ is consistent, for n large enough $\boldsymbol{\beta}^* \in \mathscr{B}_0$. For such n,

$$\frac{1}{n}\sum_{i=1}^{n} \left\| h'(Y_i, \boldsymbol{X}_i, \boldsymbol{\beta}^*) \right\| \leq \frac{1}{n}\sum_{i=1}^{n} C(Y_i, \boldsymbol{X}_i) \xrightarrow{\mathsf{P}} \mathsf{E}\, C(Y_i, \boldsymbol{X}_i) < \infty.$$

This completes the proof. □

2.6. Deviance

Definition 2.7. The statistic

$$D(\boldsymbol{Y}, \widehat{\boldsymbol{\beta}}_n) = 2\varphi_0 \big[\widetilde{\ell}_n(\boldsymbol{Y}) - \ell_n(\widehat{\boldsymbol{\beta}}_n \mid \boldsymbol{Y}) \big],$$

where $\widetilde{\ell}_n(\boldsymbol{Y})$ is the maximized log-likelihood of the saturated model, is called *the (unscaled) deviance* of the model with parameters $\boldsymbol{\beta}_0 \in \mathbb{R}^p$ and observations $\boldsymbol{Y}$. ▽

Note. In the saturated model, the MLE of μ_i is Y_i (see p. 22) and the MLE of θ_i is $\widetilde{\theta}_i = (b')^{-1}(Y_i)$. The maximized log likelihood (2.5) of the saturated model is

$$\widetilde{\ell}_n(\boldsymbol{Y}) = \frac{1}{\varphi_0}\sum_{i=1}^{n} \big[Y_i \widetilde{\theta}_i - b(\widetilde{\theta}_i) \big].$$

In the model with parameters $\boldsymbol{\beta}_0 \in \mathbb{R}^p$, the maximized log likelihood (2.5) is

$$\ell_n(\widehat{\boldsymbol{\beta}}_n \mid \boldsymbol{Y}) = \frac{1}{\varphi_0}\sum_{i=1}^{n} \big[Y_i \widehat{\theta}_i - b(\widehat{\theta}_i) \big],$$

where $\widehat{\theta}_i = (b')^{-1}(\widehat{\mu}_i)$. Obviously, $\widetilde{\ell}_n(\boldsymbol{Y}) \geq \ell_n(\widehat{\boldsymbol{\beta}}_n \mid \boldsymbol{Y})$.

The unscaled deviance can be expressed as

$$D(\boldsymbol{Y}, \widehat{\boldsymbol{\beta}}_n) = 2\sum_{i=1}^{n} \big[Y_i(\widetilde{\theta}_i - \widehat{\theta}_i) - b(\widetilde{\theta}_i) + b(\widehat{\theta}_i) \big]. \tag{2.12}$$

The deviance is always non-negative, does not depend on φ_0, and is zero if and only if the model provides a "perfect fit".

Note.

- The deviance is a goodness-of-fit measure. When the data are normal, the deviance is equal to the residual sums of squares. It generalizes the term residual sums of squares to the GLM*.
- $D^*(\boldsymbol{Y}, \widehat{\boldsymbol{\beta}}_n, \varphi_0) = \varphi_0^{-1} D(\boldsymbol{Y}, \widehat{\boldsymbol{\beta}}_n)$ is called *the scaled deviance*. If φ_0 is unknown, use the moment estimator $\widehat{\varphi}_n$ defined by (2.11).

The end of lecture 6 (Mar. 18)

2.7. Asymptotic Results

Asymptotic results for the GLM follow from the general theory of maximum likelihood estimation. The theory is reviewed in the Appendix starting on p. 62.

The following theorem transcribes the results of Theorems A.2 – A.5 from the Appendix in the context of the GLM. The regularity conditions R1 – R4 are assured by the specification of the model. Condition R6 has been verified in Theorem 2.3, part (i) and Theorem 2.4, part (ii).

The Fisher information matrix

$$I(\boldsymbol{\beta}_0) = \mathsf{E}\, I(\boldsymbol{\beta}_0 \mid Y_i) = \operatorname{var} \boldsymbol{U}(\boldsymbol{\beta}_0 \mid Y_i) = \frac{1}{\varphi_0} \mathsf{E}_{\boldsymbol{X}} w(\mu_i) \boldsymbol{X}_i^{\otimes 2}$$

is finite and of full rank by assumptions imposed on the covariates (finiteness of all necessary moments and linear independence of covariates).

Theorem 2.7.

(i) The MLE $\widehat{\boldsymbol{\beta}}_n$ is consistent (as long as the likelihood equations (2.7) have a unique solution).

(ii)

$$\frac{1}{\sqrt{n}} \boldsymbol{U}_n(\boldsymbol{\beta}_0) \xrightarrow{D} N_p(\boldsymbol{0}, I(\boldsymbol{\beta}_0)).$$

(iii)

$$\sqrt{n}(\widehat{\boldsymbol{\beta}}_n - \boldsymbol{\beta}_0) \xrightarrow{D} N_p(\boldsymbol{0}, I^{-1}(\boldsymbol{\beta}_0)).$$

(iv)

$$2 \log \frac{L_n(\widehat{\boldsymbol{\beta}}_n \mid \boldsymbol{Y})}{L_n(\boldsymbol{\beta}_0 \mid \boldsymbol{Y})} \xrightarrow{D} \chi^2_p.$$

♢

* The Pearson X^2 is another generalization.

The information matrix $I(\boldsymbol{\beta}_0)$ can be consistently estimated by

$$\widehat{I}_n = \frac{1}{n\widehat{\varphi}_n}\mathbb{X}^{\mathsf{T}}\hat{\mathbb{W}}\mathbb{X}.$$

According to part (iii) of Theorem 2.7, the estimated asymptotic variance of $\widehat{\boldsymbol{\beta}}_n$ is

$$\widehat{I}_n^{-1}/n = \widehat{\varphi}_n(\mathbb{X}^{\mathsf{T}}\hat{\mathbb{W}}\mathbb{X})^{-1}. \tag{2.13}$$

Denote $\widehat{\Sigma} \equiv (\mathbb{X}^{\mathsf{T}}\hat{\mathbb{W}}\mathbb{X})^{-1}$ so that $\widehat{\varphi}_n\widehat{\Sigma}$ estimates $\mathsf{var}\,\widehat{\boldsymbol{\beta}}_n$.

Let us consider the problem of testing the simple hypothesis

$$H_0 : \boldsymbol{\beta} = \boldsymbol{\beta}_0 \qquad \text{against} \qquad H_1 : \boldsymbol{\beta} \neq \boldsymbol{\beta}_0.$$

The test statistics and their null distributions are established by the following theorem, which is based on Definition A.5 and Theorem A.7 from the Appendix.

Theorem 2.8.

(i) ***Score (Rao) test.*** *Let* $\mu_i^0 = g^{-1}(\boldsymbol{X}_i^T\boldsymbol{\beta}_0)$, $\mathbb{W}^0 = \mathrm{diag}\,(w(\mu_1^0),\dots,w(\mu_n^0))$, *denote* $\Sigma^0 = (\mathbb{X}^T\mathbb{W}^0\mathbb{X})^{-1}$. *If* H_0 *holds then*

$$\begin{aligned} R_n &= \frac{1}{n}\boldsymbol{U}_n(\boldsymbol{\beta}_0)^T\widehat{I}_n^{-1}\boldsymbol{U}_n(\boldsymbol{\beta}_0) \\ &= \frac{1}{\widehat{\varphi}_n}\Big(\sum_{i=1}^n w(\mu_i^0)g'(\mu_i^0)(Y_i-\mu_i^0)\boldsymbol{X}_i\Big)^T\Sigma^0\Big(\sum_{i=1}^n w(\mu_i^0)g'(\mu_i^0)(Y_i-\mu_i^0)\boldsymbol{X}_i\Big) \\ &\xrightarrow{D} \chi^2_p \end{aligned}$$

(ii) ***Wald test.*** *If* H_0 *holds then*

$$W_n = n\big(\widehat{\boldsymbol{\beta}}_n-\boldsymbol{\beta}_0\big)^T\widehat{I}_n\big(\widehat{\boldsymbol{\beta}}_n-\boldsymbol{\beta}_0\big) = \frac{1}{\widehat{\varphi}_n}\big(\widehat{\boldsymbol{\beta}}_n-\boldsymbol{\beta}_0\big)^T\widehat{\Sigma}^{-1}\big(\widehat{\boldsymbol{\beta}}_n-\boldsymbol{\beta}_0\big) \xrightarrow{D} \chi^2_p$$

(iii) ***Likelihood ratio test.*** *Let* $\theta_i^0 = (b')^{-1}(\mu_i^0)$. *If* H_0 *holds then*

$$\lambda_n = 2[\ell_n(\widehat{\boldsymbol{\beta}}_n \mid \boldsymbol{Y}) - \ell_n(\boldsymbol{\beta}_0 \mid \boldsymbol{Y})] = \frac{2}{\widehat{\varphi}_n}\sum_{i=1}^n\big[Y_i(\widehat{\theta}_i-\theta_i^0) - b(\widehat{\theta}_i) + b(\theta_i^0)\big] \xrightarrow{D} \chi^2_p \quad \diamondsuit$$

The simple hypothesis is rarely of interest for applications. We are more interested in composite hypotheses, for example, in testing that the last m components of the regression parameter vector are all zero (without loss of generality: the components of $\boldsymbol{\beta}$ can be always rearranged in this way). Take

$$H_0^* : \begin{pmatrix}\beta_{p-m+1}\\ \beta_{p-m+2}\\ \vdots \\ \beta_p\end{pmatrix} = \mathbf{0} \qquad \text{against} \qquad H_1^* : \begin{pmatrix}\beta_{p-m+1}\\ \beta_{p-m+2}\\ \vdots \\ \beta_p\end{pmatrix} \neq \mathbf{0}$$

for some $m < p$. If H_0^* is true then the last m parameters attain zero value and the last m components of the covariate vector can be excluded from the model. The null hypothesis specifies a submodel (with $p-m$ parameters) of the full model with (p parameters).

Denote $\boldsymbol{\beta}_M = (\beta_{p-m+1}, \ldots, \beta_p)^\mathsf{T}$ and $\boldsymbol{X}_i^M = (X_{i,p-m+1}, \ldots, X_{ip})^\mathsf{T}$. Let $\widehat{\boldsymbol{\beta}}_M = (\widehat{\beta}_{p-m+1}, \ldots, \widehat{\beta}_p)^\mathsf{T}$ be the MLE of $\boldsymbol{\beta}_M$ under the larger model. Let $\widetilde{\boldsymbol{\beta}}_n$ be the MLE of $\boldsymbol{\beta}$ under the submodel (subject to the constraint $\boldsymbol{\beta}_M = \mathbf{0}$), let $\widetilde{\mu}_i = g^{-1}(\boldsymbol{X}_i^\mathsf{T}\widetilde{\boldsymbol{\beta}}_n)$ be the fitted values under the submodel.

Partition the $p \times p$ matrix $\widehat{\Sigma} = \widehat{I}_n^{-1}/(n\widehat{\varphi}_n) = (\mathbb{X}^\mathsf{T}\widehat{\mathbb{W}}\mathbb{X})^{-1}$ (the estimated asymptotic variance of $\widehat{\boldsymbol{\beta}}_n$ without $\widehat{\varphi}_n$) into four blocks

$$\widehat{\Sigma} = \begin{pmatrix} \widehat{\Sigma}_A & \widehat{\Sigma}_B \\ \widehat{\Sigma}_B^\mathsf{T} & \widehat{\Sigma}_M \end{pmatrix},$$

where the lower right block $\widehat{\Sigma}_M$ is of size $m \times m$.

Theorem 2.9.

(i) ***Score (Rao) test.*** *Let $\widetilde{\mathbb{W}} = \operatorname{diag}(w(\widetilde{\mu}_1), \ldots, w(\widetilde{\mu}_n))$. Let $\widetilde{\Sigma}_M$ be the $m \times m$ lower right block of the matrix $\widetilde{\Sigma} = (\mathbb{X}^T\widetilde{\mathbb{W}}\mathbb{X})^{-1}$. Denote by $\widetilde{\varphi}_n$ the estimator of the dispersion parameter calculated under the submodel (under H_0^*). If H_0^* holds then*

$$R_n^* = \frac{1}{\widetilde{\varphi}_n}\left(\sum_{i=1}^n w(\widetilde{\mu}_i)g'(\widetilde{\mu}_i)(Y_i - \widetilde{\mu}_i)\boldsymbol{X}_i^M\right)^T \widetilde{\Sigma}_M \left(\sum_{i=1}^n w(\widetilde{\mu}_i)g'(\widetilde{\mu}_i)(Y_i - \widetilde{\mu}_i)\boldsymbol{X}_i^M\right) \xrightarrow{D} \chi_m^2.$$

(ii) ***Wald test.*** *Denote by $\widehat{\varphi}_n$ the estimator of the dispersion parameter calculated under the larger model (not assuming that H_0^* is true). If H_0^* holds then*

$$W_n^* = \frac{1}{\widehat{\varphi}_n}\big(\widehat{\boldsymbol{\beta}}^M\big)^T \widehat{\Sigma}_M^{-1}\big(\widehat{\boldsymbol{\beta}}^M\big) \xrightarrow{D} \chi_m^2.$$

(iii) ***Likelihood ratio (deviance) test.*** *Let $D(\boldsymbol{Y} \mid \widetilde{\boldsymbol{\beta}})$ be the (unscaled) deviance of the submodel, let $D(\boldsymbol{Y} \mid \widehat{\boldsymbol{\beta}})$ be the (unscaled) deviance of the larger model. Let the estimate $\widehat{\varphi}_n$ be calculated under the larger model (not assuming that H_0^* is true). If H_0^* holds then*

$$\lambda_n^* = \frac{1}{\widehat{\varphi}_n}\big[D(\boldsymbol{Y} \mid \widetilde{\boldsymbol{\beta}}) - D(\boldsymbol{Y} \mid \widehat{\boldsymbol{\beta}})\big] \xrightarrow{D} \chi_m^2. \qquad \diamondsuit$$

Note.

- Theorem 2.9 follows from Definition A.6 and Theorem A.9 in the Appendix. The hypothesis H_0^* is rejected at the asymptotic level of α if the chosen test statistic (it must be selected in advance) exceeds the $1-\alpha$ quantile of the χ_m^2 distribution.

- Under the standard linear regression model with normal distribution, these three test statistics are all equal to the F test statistic (1.1) for submodel testing. In that case, the exact distribution of the test statistics under the null hypothesis is $F_{m,n-p}$. When normality does not hold or the link is not identity, the three test statistics are not the same and we only know that their asymptotic distribution is χ^2_m.
- Generally, the likelihood ratio test statistic is twice the difference in the log likelihoods between the model and the submodel. However, it can be also expressed as a properly scaled difference in deviances between the submodel and the model. *The deviance test is the preferred tool for testing submodels in generalized linear models.*
- The Wald and Rao statistics are asymptotically equivalent to the likelihood ratio test statistic. However, in finite samples they may be different. Unlike the likelihood ratio test statistic, the Wald test statistic depends on the parametrization of the model and tends to have the slowest convergence to the asymptotic distribution. For these reasons, the Wald statistic is the least desirable of the three.
- An important special case is $m = 1$ (testing of a single parameter). Then the Wald statistic for testing zero value of the j-th parameter is

$$\left(\frac{\widehat{\beta}_j}{\sqrt{\widehat{\varphi}_n \widehat{\sigma}^2_{jj}}}\right)^2, \tag{2.14}$$

  where $\widehat{\sigma}^2_{jj}$ is the j-th diagonal element of $\widehat{\Sigma}$. Before applying the square, these statistics are asymptotically standard normal; in this form they are automatically provided in the output of almost any statistical software for fitting the GLM.
- The deviance of the current model $D(\boldsymbol{Y} \mid \widehat{\boldsymbol{\beta}})$ is twice the difference in log likelihoods between the saturated model and the current model. However, the deviance cannot be in general used as a test statistic to compare the goodness-of-fit of the current model to the saturated model unless all covariates are discrete (otherwise the number of parameters of the saturated model grows to infinity and Theorem A.9 from *MLE Summary* does not hold). Differences in deviances between a submodel and a larger model do not have this problem.

Confidence intervals

The simplest confidence intervals for the individual parameters are based on Wald test statistics (2.14). The interval with end points

$$\widehat{\beta}_j \pm u_{1-\alpha/2}\sqrt{\widehat{\varphi}_n \widehat{\sigma}^2_{jj}},$$

covers β_j with probability converging to $1-\alpha$.

Better confidence intervals would be obtained from inverting acceptance regions of the Rao or likelihood ratio test statistics or using profile likelihood methods.

Wald-type confidence intervals for linear combinations of parameters $\boldsymbol{c}^\mathsf{T}\boldsymbol{\beta}_0$ where $\mathbf{0} \neq \boldsymbol{c} \in \mathbb{R}^p$ can be obtained easily from Theorem 2.7 part (iii). An asymptotic confidence interval with coverage probability converging to $1-\alpha$ is

$$\boldsymbol{c}^\mathsf{T}\widehat{\boldsymbol{\beta}}_n \pm u_{1-\alpha/2}\sqrt{\widehat{\varphi}_n \boldsymbol{c}^\mathsf{T}\widehat{\Sigma}\boldsymbol{c}}.$$

The end of lecture 7 (Mar. 22)

2.8. Diagnostic Methods for the GLM

Diagnostic methods can be derived from the linear model using Theorem 2.5. Let $\mathbb{X}^* = \hat{\mathbb{W}}^{1/2}\mathbb{X}$ and $\boldsymbol{Y}^* = \hat{\mathbb{W}}^{1/2}\widehat{\boldsymbol{Z}}$. Recall that $\hat{\mathbb{W}} = \operatorname{diag}(w(\widehat{\mu}_1), \ldots, w(\widehat{\mu}_n))$ and

$$\widehat{Z}_i = \widehat{\eta}_i + (Y_i - \widehat{\mu}_i)g'(\widehat{\mu}_i).$$

Write $\widehat{\boldsymbol{\beta}}_n$ as an ordinary least squares estimator $\widehat{\boldsymbol{\beta}}_n = (\mathbb{X}^{*\mathsf{T}}\mathbb{X}^*)^{-1}\mathbb{X}^{*\mathsf{T}}\boldsymbol{Y}^*$. Let

$$\mathbb{H}^* = \mathbb{X}^*(\mathbb{X}^{*\mathsf{T}}\mathbb{X}^*)^{-1}\mathbb{X}^{*\mathsf{T}} = \hat{\mathbb{W}}^{1/2}\mathbb{X}(\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}\mathbb{X})^{-1}\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}^{1/2},$$

and $\hat{\boldsymbol{Y}}^* = \mathbb{X}^*\widehat{\boldsymbol{\beta}} = \mathbb{H}^*\boldsymbol{Y}^* = \hat{\mathbb{W}}^{1/2}\mathbb{X}(\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}\mathbb{X})^{-1}\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}\widehat{\boldsymbol{Z}}$.

2.8.1. Pearson residuals

Pearson residuals are defined by the identity $\boldsymbol{r}^P = \boldsymbol{Y}^* - \hat{\boldsymbol{Y}}^* = \hat{\mathbb{W}}^{1/2}\widehat{\boldsymbol{Z}} - \hat{\mathbb{W}}^{1/2}\mathbb{X}\widehat{\boldsymbol{\beta}}$, which gives the following residuals for the individual observations

$$r_i^P = \frac{Y_i - \widehat{\mu}_i}{\sqrt{V(\widehat{\mu}_i)}}.$$

Sum of squares of Pearson residuals is equal to the Pearson X^2 statistic:

$$\sum_{i=1}^{n}\left(r_i^P\right)^2 = X^2.$$

We have $\boldsymbol{r}^P = (\mathbb{I}_n - \mathbb{H}^*)\boldsymbol{Y}^*$ and

$$\operatorname{var}\boldsymbol{Y}^* \doteq \mathbb{W}^{1/2}\operatorname{var}\boldsymbol{Z}\,\mathbb{W}^{1/2} = \mathbb{W}^{1/2}\operatorname{diag}(\varphi_0 V(\mu_i)[g'(\mu_i)]^2)\mathbb{W}^{1/2} = \varphi_0\mathbb{I}_n.$$

Because $\mathbb{I}_n - \mathbb{H}^*$ is idempotent,

$$\operatorname{var}\boldsymbol{r}^P \doteq \varphi_0(\mathbb{I}_n - \mathbb{H}^*).$$

2.8.2. Leverages

It has been shown above that

$$\mathsf{var}\, r_i^P \doteq \varphi_0(1-h_{ii}^*),$$

where h_{ii}^*, the i-th diagonal element of $\mathbb{H}^*$, is called *the leverage*. Potentially influential observations can be identified by the rule of thumb $h_{ii}^* > 2p/(n-2p)$. These observations are sort of atypical in their covariates and thus may have unduly strong influence on the results of the model fit.

2.8.3. Standardized Pearson residuals

Standardized Pearson residuals normalize r_i^P by division by the square root of its approximate variance:

$$r_i^{PS} = \frac{Y_i - \widehat{\mu}_i}{\sqrt{\widehat{\varphi}_n V(\widehat{\mu}_i)(1-h_{ii}^*)}}.$$

They have approximately unit variance.

2.8.4. Deviance residuals

Deviance residuals are signed square roots of the contributions of the observations to the deviance. Let $\widetilde{\theta}_i = (b')^{-1}(Y_i)$, $d_i = 2\big\{Y_i[\widetilde{\theta}_i - \widehat{\theta}_i] - b(\widetilde{\theta}_i) + b(\widehat{\theta}_i)\big\}$, and define the deviance residual as

$$r_i^D = \operatorname{sgn}(Y_i - \widehat{\mu}_i)\sqrt{d_i}.$$

Sum of squares of deviance residuals is equal to the deviance:

$$\sum_{i=1}^{n} \big(r_i^D\big)^2 = D(\boldsymbol{Y} \mid \widehat{\boldsymbol{\beta}}).$$

2.8.5. Standardized deviance residuals

Standardized deviance residuals use the same normalization as standardized Pearson residuals.

$$r_i^{DS} = \frac{\operatorname{sgn}(Y_i - \widehat{\mu}_i)\sqrt{d_i}}{\sqrt{\widehat{\varphi}_n(1-h_{ii}^*)}}.$$

These are the default residuals in R.

2.8.6. Cook's distance

Cook's distance measures the influence of the i-th observation on the estimates of regression parameters $\widehat{\boldsymbol{\beta}}$. Let $\widehat{\boldsymbol{\beta}}_{(i)}$ denote the estimates calculated after deletion of the i-th observation from the data set. Cook's distance is defined as

$$CD_i = \frac{1}{p\widehat{\varphi}_n}(\widehat{\boldsymbol{\beta}} - \widehat{\boldsymbol{\beta}}_{(i)})^{\mathsf{T}}\mathbb{X}^{*\mathsf{T}}\mathbb{X}^{*}(\widehat{\boldsymbol{\beta}} - \widehat{\boldsymbol{\beta}}_{(i)}).$$

In linear regression, it can be shown that

$$CD_i = \frac{1}{p\widehat{\varphi}_n}\left(\frac{Y_i^* - \hat{Y}_i^*}{\sqrt{1-h_{ii}^*}}\right)^2 \frac{h_{ii}^*}{1-h_{ii}^*} = \frac{1}{p}\left(r_i^{PS}\right)^2 \frac{h_{ii}^*}{1-h_{ii}^*}.$$

This is how Cook's distance is calculated in the GLM. An observation is considered influential if $CD_i > \frac{8}{n-2p}$.

2.8.7. Residual plots

Residual plots are created and used in a direct analogy with the linear model. However, for some data types (e.g. binary data) the residual plots are much less informative and require smoothing to yield any useful information. In general, residual plots are somewhat less useful in the GLM than they are in the linear model.

2.8.8. Diagnostics of the link function

We only mention two simple methods for checking that the correct link function was selected. Plotting the adjusted dependent variable $\widehat{Z}_i$ against the linear predictor $\widehat{\eta}_i$ provides a graphical check. If the link is correct the plot should reveal a linear pattern. A formal test can be obtained by adding $(\widehat{\eta}_i)^2$ to the model as an additional covariate and testing that its parameter is zero. If the hypothesis is rejected the link may be incorrect.

Both methods are sensitive to inappropriate transformations of the regressors. If the transformations are not chosen well, both methods may indicate a problem even if the link is correct.

Incorrect link functions do not have a serious effect on deciding which regressors affect the response or on the results of submodel testing. The choice of the link function is important if the primary goal of the analysis is prediction.

2.9. Model-building strategies

Model-building strategies for generalized linear models do not differ from the strategies applied to other regression models, including linear regression. The primary tool for model

building are deviance tests comparing a larger model with a submodel. If the deviance test is significant it means that the terms in the larger model cannot be removed without a significant decrease in the quality of model fit.

Since the development of the final model usually involves repeated applications of deviance tests, each performed on a selected level α (usually $\alpha = 0.05$), it is clear that the overall procedure does not preserve the desired level. If many tests are done then the final model is likely to include terms that in fact do not affect the response at all (*overfitting*). There is no universal and reliable method for adjusting the levels of the individual tests so that the overall probability of including irrelevant terms is under control. Nevertheless the analyst should be aware of this problem and should not interpret the p-values of submodel tests too dogmatically.

Approaches for developing reasonable models vary with the nature of the problem, structure of the data and questions to be addressed by the analysis. There is no universal solution to be recommended. Each problem requires careful consideration by the analyst taking into account the nature of the problem, the data-collection methods and tools, the meaning of the variables included in the dataset, their mutual relationships, and the goals of the analysis.

If *prediction* is the primary goal, it is useful to consider rich and flexible models. Omission of an important term from the model or its inclusion with an inappropriate transformation may have detrimental biasing effects on the predictions. If unnecessary covariates are left in, the variability in the predicted response is increased but the predictions are not biased. Interpretation of regression parameters is usually not that important. In prediction analyses, validation of the prediction model should be performed either by dividing the data set into disjoint training (used for model building) and validation (used for evaluation of the predictions) subsets or at least by cross-validation (predictions of each observation by a model fitted on data excluding that observation). Validation is a very useful tool for selection of the best prediction model out of several candidates.

If the goal is to *evaluate covariate effects* ("how does covariate X affect the mean of the response Y?"), one must be really careful about several things. First, the covariate of interest must be kept in the model even if it is not significant – otherwise its effect cannot be evaluated. Second, the regression parameters expressing the influence of the covariate of interest should have a straightforward interpretation. Thus, we cannot afford to model the effect of X by a complicated function that cannot be easily summarized (splines of order > 1, polynomials), or to use complex transformations of the response or link functions that are difficult to interpret. Third, there might be covariates that should be kept in the model regardless of their significance (suspected confounders) and/or covariates that should not be included in the model no matter how significant they are (variables on the causal pathway between X and Y, variables that are influenced by the value of Y). Thus, making reasonable decisions about which covariates should be included in the model and which should be dropped is not based solely on significance tests but also on external expert knowledge of the problem to be analyzed. It is precisely this issue that makes automated computer-based algorithms

(unsupervised stepwise regression, regression trees, neural networks, deep learning, etc.) unable to solve certain problems acceptably.

Another common problem in model-building strategies is the inclusion of *interactions*, especially when the number of covariates that can be considered for interactions is quite large. The strategy that starts with a model that includes a lot of main effects as well as all possible two-way interactions between them, and tries to gradually eliminate the superfluous terms usually does not lead to a good model. With this approach, we are likely to end up with a model that suffers from overfitting, keeps a lot of unnecessary interactions and is hard to interpret. It is better to fit only the main effects first, eliminate those that are not contributing to the model, and then try to add two-way interactions of the remaining terms one by one. This strategy is much more likely to end up only with interactions that really matter. Considering higher order interactions (three-way, four-way,...) is usually a hopeless task. It is better not to consider them at all, except in analyses where, for some reason, such interactions are among the terms of interest.

There is one principle about building models with interactions, which is almost universally valid and the analyst should take care not to violate it. The models should be built *hierarchically*, meaning that if a covariate is present in a higher-order interaction, then all its corresponding lower-order interactions as well as the main effects should be included in the model as well, no matter if they are significant or not. This principle should be ignored only in analyses where there is a sound justification for its violation.

This brief exposition of model-building strategies cannot be complete and should be understood in the whole context of the particular task to be done. As noted earlier, each problem should be carefully considered in order to choose a tailor-made strategy that works well for it. This requires practical experience. The analyst should be aware that there is no such thing as the true model and that his task is not to discover it. All models are wrong – we are only looking for an acceptable model that provides satisfactory answers to the questions of interest.

The end of lecture 8 (Mar. 22)

3. Generalized Linear Model for Discrete Responses

3.1. Analysis of Binary Data

3.1.1. Alternative vs. binomial data

Let $Y_{ij}^* \sim \mathsf{Alt}(\pi_i)$, $\pi \in (0,1)$, be independent variables for $i = 1,\dots,K$, $j = 1,\dots,m_i$. For a fixed i, $Y_{i1}^*,\dots,Y_{im_i}^*$ are identically distributed. The total number of observations is $N = \sum_{i=1}^{K} m_i$. Let π_i depend on $\boldsymbol{X}_i = (X_{i1},\dots,X_{ip})^\mathsf{T}$ through the linear predictor $\eta_i = \boldsymbol{X}_i^\mathsf{T}\boldsymbol{\beta}$, $\boldsymbol{\beta}$ is the vector of unknown regression coefficients to be estimated. Therefore $Y_{i1}^*,\dots,Y_{im_i}^*$ share the same covariate vector $\boldsymbol{X}_i$.

The response $Y_{ij}^* \sim \mathsf{Alt}(\pi_i)$ has a distribution of exponential family with $\mu_i \equiv \mathsf{E}\, Y_{ij}^* = \pi_i$ and $\mathsf{var}\, Y_{ij}^* = \pi_i(1-\pi_i)$. The variance function is $V(\mu) = \mu(1-\mu)$, the dispersion parameter is $\varphi = 1$, the canonical parameter is $\theta_i = \log\frac{\pi_i}{1-\pi_i}$. Finally, $b(\theta_i) = \log(1+\mathrm{e}^{\theta_i}) = \log\frac{1}{1-\pi_i}$.

Denote $Y_i = \sum_{j=1}^{m_i} Y_{ij}^*$. Then $Y_i \sim \mathsf{Bi}(m_i,\pi_i)$. Because a binomial response can be always written as a sum of independent responses with an alternative distribution, the GLM developed for the alternative distribution can be also used to fit regression models to binomial responses even though the binomial distribution does not strictly belong to the exponential family as we defined it.

The dataset with alternative or binomial responses can be arranged in two different formats (see Figure 3.1) that can be transformed one to the other.

Format A. The dataset is arranged so that there are N rows corresponding to the alternative responses Y_{ij}^* and each value of the covariate vector $\boldsymbol{X}_i$ appears in m_i different rows. The row corresponding to the ij-th observation includes Y_{ij}^* and $\boldsymbol{X}_i$. This will be called *the Bernoulli format* of the data or *the alternative format*.

Format B. The dataset is arranged so that there are K rows corresponding to the binomial responses Y_i and each value of $\boldsymbol{X}_i$ appears only once in the whole dataset. The i-th row includes Y_i, m_i, and $\boldsymbol{X}_i$. This will be called *the binomial format* of the data.

Note. It is a bad idea to mix the two data formats in a single dataset.

Note. If the covariate vector has at least one continuous component (with no rounding) then $m_i = 1$ for all i, $N = K$ and the two data formats are the same.

Figure 3.1.: Binary data written in the alternative format A (left panel) vs. the binomial format B (right panel).

Format A.

$$\left.\begin{matrix} Y^*_{11} & \boldsymbol{X}_1^\top \\ \vdots & \vdots \\ Y^*_{1m_1} & \boldsymbol{X}_1^\top \end{matrix}\right\} m_1 \times$$

$$\vdots$$

$$\left.\begin{matrix} Y^*_{K1} & \boldsymbol{X}_K^\top \\ \vdots & \vdots \\ Y^*_{Km_K} & \boldsymbol{X}_K^\top \end{matrix}\right\} m_K \times$$

Format B.

$$\left.\begin{matrix} Y_1 & m_1 & \boldsymbol{X}_1^\top \\ Y_2 & m_2 & \boldsymbol{X}_2^\top \\ \vdots & \vdots & \vdots \\ Y_K & m_K & \boldsymbol{X}_K^\top \end{matrix}\right\} K \times$$

The presence or absence of at least one continuous covariate leads to one of two different kinds of asymptotics when $N \to \infty$.

1. When all covariates are discrete with a finite support then K is constant, and $m_i \to \infty$ at the same rate for all i.
2. When at least one covariate is continuous then $K \to \infty$ and all m_i are small (typically $m_i = 1$).

Most of the results are the same for both data formats and both kinds of asymptotics but there are certain important differences that will be pointed out later.

3.1.2. Link functions for binary data

Because $\mu_i \equiv \pi_i \in (0,1)$, suitable link functions are maps $(0,1) \to \mathbb{R}$. Any quantile function of a continuous distribution on $\mathbb{R}$ could be used as a link function for binary responses. Here are some examples:

Logistic link

Take the quantile function of the standard logistic distribution.

$$g(\mu_i) = \log \frac{\mu_i}{1-\mu_i}, \qquad \mu_i = \frac{\exp\{\boldsymbol{X}_i^\top \boldsymbol{\beta}\}}{1+\exp\{\boldsymbol{X}_i^\top \boldsymbol{\beta}\}}.$$

This is the logistic link, the canonical link function, the most commonly used link for binary data. The model is called *the logistic regression model*[*].

[*] Česky *logistická regrese*

Probit link

Take the quantile function of the standard normal distribution.

$$g(\mu_i) = \Phi^{-1}(\mu_i), \qquad \mu_i = \Phi(\boldsymbol{X}_i^\top \boldsymbol{\beta}).$$

This is the probit link, the model is called *the probit regression model*[*]. It is used in threshold analysis, toxicology and pharmacokinetics.

Cauchit link

Take the quantile function of the standard Cauchy distribution.

$$g(\mu_i) = \tan[\pi(\mu_i - 0.5)], \qquad \mu_i = \frac{1}{\pi}\arctan(\boldsymbol{X}_i^\top \boldsymbol{\beta}) + \frac{1}{2}.$$

This is the cauchit link, the model is called *the cauchit regression model*[†]. It is suitable when π_i converges to 0 (1) extremely slowly for $\eta_i \to \pm\infty$.

Complementary log-log link

Take the quantile function of the negative Gumbel (extreme value) random variable.

$$g(\mu_i) = \log(-\log(1-\mu_i)), \qquad \mu_i = 1 - \mathrm{e}^{-\exp\{\boldsymbol{X}_i^\top \boldsymbol{\beta}\}}.$$

This link function does not possess symetry properties. It is used in the analysis of discrete survival data. Its counterpart is the log-log link

$$g(\mu_i) = -\log(-\log(\mu_i)), \qquad \mu_i = \mathrm{e}^{-\exp\{-\boldsymbol{X}_i^\top \boldsymbol{\beta}\}}.$$

The inverse link functions are plotted in Figure 3.2. The choice of the link function should be governed by the desired interpretation of the fitted model rather than by the data. The canonical logistic link should be the first choice unless a different interpretation is needed or there is a strong prior reason to choose a different link.

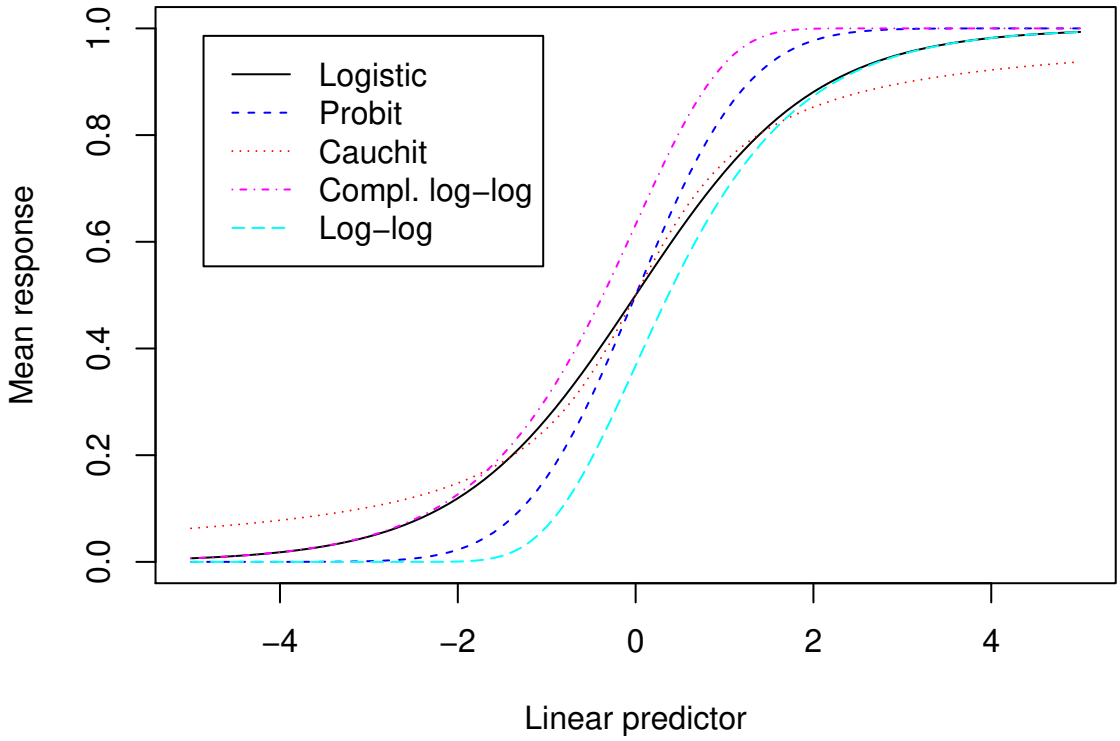
3.1.3. Binary data likelihood

There are two different sampling schemes to be considered.

(i) Alternative responses are observed independently of each other together with the covariates. Then m_i are random variables.

[*] Česky *probitová regrese* [†] Česky *cauchitová regrese*

Figure 3.2.: Inverse link functions for binary data. The linear predictor η_i is on the horizontal axis, the success probability π_i is on the vertical axis.



(ii) m_i is fixed in advance, then m_i independent observations are obtained for each combination of the covariates.

The likelihoods for these two schemes only differ by a constant that does not affect the analysis. If m_i is random then the likelihood is a product of independent alternative distributions

$$\prod_{i=1}^{K}\prod_{j=1}^{m_i}\pi_i^{Y_{ij}^*}(1-\pi_i)^{1-Y_{ij}^*}=\prod_{i=1}^{K}\pi_i^{Y_i}(1-\pi_i)^{m_i-Y_i}.$$

If m_i is fixed then the likelihood is a product of independent binomial distributions

$$\prod_{i=1}^{K}\binom{m_i}{Y_i}\pi_i^{Y_i}(1-\pi_i)^{m_i-Y_i}=\prod_{i=1}^{K}\pi_i^{Y_i}(1-\pi_i)^{m_i-Y_i}\prod_{i=1}^{K}\binom{m_i}{Y_i}.$$

The product of the binomial numbers does not include the parameters, so it is not relevant. The first scheme follows the framework of independent observations from a distribution of exponential type so the theory of Chapter 2 applies. The second scheme does not follow the

framework of Chapter 2 strictly but the core of the likelihood is the same and all the results have exactly the same form and properties. Therefore we do not have to distinguish the two sampling schemes.

3.1.4. Threshold analysis by probit regression

The probit link has an interesting application in threshold analysis of normally distributed data.

Consider random variables U_i that follow the normal linear regression model

$$U_i = \boldsymbol{Z}_i^\top \boldsymbol{\alpha} + \varepsilon_i, \tag{3.1}$$

where $\boldsymbol{Z}_i$ are p-dimensional covariate vectors, $\boldsymbol{\alpha}$ are regression coefficients and $\varepsilon_i \sim \mathsf{N}(0, \sigma^2)$ are error terms. Now suppose that the responses U_i cannot be observed directly. Instead, a threshold C_i is provided and we learn whether the unobserved response U_i exceeds the threshold or not.

Assume that C_i is independent of U_i. The observed response is $Y_i = \mathbb{1}(U_i < C_i)$, together with the values of the covariates $\boldsymbol{Z}_i$ and the threshold C_i. The goal is to estimate the regression coefficients α and the residual variance σ^2 of the underlying linear regression model (3.1).

The observations come in the form of iid triplets $(Y_i, C_i, \boldsymbol{Z}_i)$. The response Y_i follows an alternative distribution with

$$\mathrm{P}[Y_i = 1] \equiv p_i = \mathrm{P}[U_i < C_i].$$

Conditionally on the value of the observed threshold C_i, we get

$$p_i = \mathrm{P}\left[\frac{U_i - \boldsymbol{Z}_i^\top \boldsymbol{\alpha}}{\sigma} < \frac{C_i - \boldsymbol{Z}_i^\top \boldsymbol{\alpha}}{\sigma}\right] = \Phi\left(\frac{C_i}{\sigma} - \boldsymbol{Z}_i^\top \frac{\boldsymbol{\alpha}}{\sigma}\right).$$

Define

$$\boldsymbol{X}_i = \begin{pmatrix} \boldsymbol{Z}_i \\ C_i \end{pmatrix} \quad \text{and} \quad \boldsymbol{\beta} = \begin{pmatrix} -\boldsymbol{\alpha}/\sigma \\ 1/\sigma \end{pmatrix}.$$

This translates the problem into binary probit regression model with the linear predictor $\boldsymbol{X}_i^\top \boldsymbol{\beta}$. The parameters $\boldsymbol{\beta}$ can be estimated by the usual procedures for the analysis of the GLM. The parameters of interest can be obtained from $\widehat{\boldsymbol{\beta}}$ as $\widehat{\sigma}^2 = \frac{1}{\widehat{\beta}_{p+1}^2}$ and $\widehat{\alpha}_j = -\frac{\widehat{\beta}_j}{\widehat{\beta}_{p+1}}$.

Of course, this can only be done if the threshold values C_i are linearly independent of the covariates $\boldsymbol{Z}_i$. For example, if C_i are all set to the same value, the intercept term cannot be distinguished from the residual variance and the parameters of the original linear regression model cannot be determined.

The end of lecture 9 (Apr. 1)

3.1.5. Logistic regression

The logistic regression model is the most commonly used model for the analysis of binary and binomial responses.

The logistic link has the form $g(\pi_i) = \log \frac{\pi_i}{1-\pi_i}$, where $\pi_i/(1-\pi_i)$ is the odds of success. The success probabilities can be expressed as $\pi_i = \frac{\exp\{\boldsymbol{X}_i^\top \boldsymbol{\beta}\}}{1+\exp\{\boldsymbol{X}_i^\top \boldsymbol{\beta}\}}$.

Interpretation of regression parameters

Let $\boldsymbol{X}_i^\top \boldsymbol{\beta} = \beta_1 + \beta_2 X_2 + \cdots + \beta_p X_p$. Denote $\pi_0 = \mathrm{P}\big(Y_{ij}^* = 1 \,\big|\, X_2 = \cdots = X_p = 0\big)$. Then

$$\log \frac{\pi_0}{1-\pi_0} = \beta_1$$

so e^{β_1} is the odds of success for an individual with zero values in all covariates.

Now consider two individuals: one with observed covariates $\boldsymbol{x}^0 = (1, x_2, \ldots, x_p)^\top$, the other with observed covariates increased at the j-th component by one: $\boldsymbol{x}^j = \boldsymbol{x}^0 + \boldsymbol{e}_j$. Denote $\pi_{X0} = \mathrm{P}\big(Y_{ij}^* = 1 \,\big|\, \boldsymbol{X} = \boldsymbol{x}^0\big)$ and $\pi_{Xj} = \mathrm{P}\big(Y_{ij}^* = 1 \,\big|\, \boldsymbol{X} = \boldsymbol{x}^j\big)$. Then

$$\boldsymbol{\beta}^\top \boldsymbol{x}^0 = \log \frac{\pi_{X0}}{1-\pi_{X0}} \qquad \text{and} \qquad \boldsymbol{\beta}^\top \boldsymbol{x}^j = \boldsymbol{\beta}^\top \boldsymbol{x}^0 + \beta_j = \log \frac{\pi_{Xj}}{1-\pi_{Xj}}.$$

It follows that

$$\beta_j = \log\left(\frac{\pi_{Xj}}{1-\pi_{Xj}} \cdot \frac{1-\pi_{X0}}{\pi_{X0}} \right) \qquad \text{and} \qquad \mathrm{e}^{\beta_j} = \frac{\pi_{Xj}(1-\pi_{X0})}{\pi_{X0}(1-\pi_{Xj})}.$$

Thus e^{β_j} is the odds ratio for success comparing two individuals differing by one unit in the covariate X_j. E.g., if $\beta_j = 0.431$ one can say that a unit increase in the covariate X_j increases the odds of success $\mathrm{e}^{0.431} = 1.539$ times (or by 53.9%). When $\beta_j = 0$ the odds ratio is 1 and the covariate has no effect on the odds of success (or the probability of success) given the other covariates.

Consider a two-by-two contingency table of conditional probabilities

Covariates	$Y = 1$	$Y = 0$
$\boldsymbol{X} = \boldsymbol{x}^j$	π_{Xj}	$1-\pi_{Xj}$
$\boldsymbol{X} = \boldsymbol{x}^0$	π_{X0}	$1-\pi_{X0}$

The odds ratio e^{β_j} describes the association between $\boldsymbol{X}$ and Y in this contingency table. The odds ratio is one if and only if there is independence in this restricted table.

Estimation of parameters

By Theorem 2.3, the score statistic with the canonical link is

$$\boldsymbol{U}_n(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \sum_{i=1}^{K}\sum_{j=1}^{m_i}(Y_{ij}^* - \pi_i)\boldsymbol{X}_i = \sum_{i=1}^{K}(Y_i - m_i\pi_i)\boldsymbol{X}_i$$

and $\widehat{\boldsymbol{\beta}}_n$ solves the equations

$$\sum_{i=1}^{K} Y_i\boldsymbol{X}_i = \sum_{i=1}^{K} m_i\widehat{\pi}_i\boldsymbol{X}_i,$$

where

$$\widehat{\pi}_i = \frac{\exp\{\boldsymbol{X}_i^\mathsf{T}\widehat{\boldsymbol{\beta}}_n\}}{1+\exp\{\boldsymbol{X}_i^\mathsf{T}\widehat{\boldsymbol{\beta}}_n\}}.$$

The IWLS algorithm can be implemented in two different ways depending on the data format. With the Bernoulli format A, the regression matrix $\mathbb{X}$ includes each observed value of $\boldsymbol{X}_i$ in m_i different rows, and its dimension is $N \times p$. Suppose the observations ij are ordered by the two indices $11,\ldots,1m_1,21,\ldots,2m_2,\ldots,Km_K$. Let

$$\hat{\mathbb{W}}^{(k)} = \operatorname{diag}\big(\hat{\pi}_1^{(k)}(1-\hat{\pi}_1^{(k)}),\ldots,\hat{\pi}_K^{(k)}(1-\hat{\pi}_K^{(k)})\big)$$

be an $N \times N$ matrix, where the i-th element is repeated m_i times, define

$$\widehat{Z}_{ij}^{(k)} = \boldsymbol{X}_i^\mathsf{T}\widehat{\boldsymbol{\beta}}^{(k)} + \frac{Y_{ij}^* - \widehat{\pi}_i^{(k)}}{\widehat{\pi}_i^{(k)}(1-\widehat{\pi}_i^{(k)})},$$

and create an N-vector $\widehat{\boldsymbol{Z}}^{(k)} = (\widehat{Z}_{11}^{(k)},\ldots,\widehat{Z}_{Km_K}^{(k)})^\mathsf{T}$. The IWLS algorithm iterates

$$\widehat{\boldsymbol{\beta}}_n^{(k+1)} = (\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}^{(k)}\mathbb{X})^{-1}(\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}^{(k)}\widehat{\boldsymbol{Z}}^{(k)})$$

until convergence.

With the binomial format B, the regression matrix $\mathbb{X}_R$ includes each observed value of $\boldsymbol{X}_i$ only once, and its dimension is $K \times p$. Let

$$\hat{\mathbb{W}}_R^{(k)} = \operatorname{diag}\big(m_1\hat{\pi}_1^{(k)}(1-\hat{\pi}_1^{(k)}),\ldots,m_K\hat{\pi}_K^{(k)}(1-\hat{\pi}_K^{(k)})\big)$$

be an $K \times K$ matrix, where each element appears just once, define

$$\widehat{Z}_{Ri}^{(k)} = \boldsymbol{X}_i^\mathsf{T}\widehat{\boldsymbol{\beta}}^{(k)} + \frac{Y_i - m_i\widehat{\pi}_i^{(k)}}{m_i\widehat{\pi}_i^{(k)}(1-\widehat{\pi}_i^{(k)})},$$

and create a K-vector $\widehat{\boldsymbol{Z}}_R^{(k)} = (\widehat{Z}_{R1}^{(k)},\ldots,\widehat{Z}_{RK}^{(k)})^\mathsf{T}$. The IWLS algorithm iterates

$$\widehat{\boldsymbol{\beta}}_n^{(k+1)} = (\mathbb{X}_R^\mathsf{T}\hat{\mathbb{W}}_R^{(k)}\mathbb{X}_R)^{-1}(\mathbb{X}_R^\mathsf{T}\hat{\mathbb{W}}_R^{(k)}\widehat{\boldsymbol{Z}}_R^{(k)})$$

until convergence.

Obviously, $\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}^{(k)}\mathbb{X} = \mathbb{X}_R^\mathsf{T}\hat{\mathbb{W}}_R^{(k)}\mathbb{X}_R$ and $\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}^{(k)}\widehat{\boldsymbol{Z}}^{(k)} = \mathbb{X}_R^\mathsf{T}\hat{\mathbb{W}}_R^{(k)}\widehat{\boldsymbol{Z}}_R^{(k)}$, so the two implementations of the IWLS algorithm for the two data formats are equivalent.

The information matrix is

$$I(\boldsymbol{\beta}) = \mathsf{E}_X \widehat{\pi}_i(1-\widehat{\pi}_i)\boldsymbol{X}_i^{\otimes 2},$$

and it can be estimated by

$$\widehat{I}_n = \frac{1}{N}\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}\mathbb{X} = \frac{1}{N}\mathbb{X}_R^\mathsf{T}\hat{\mathbb{W}}_R\mathbb{X}_R.$$

The estimated variance of $\widehat{\boldsymbol{\beta}}_n$ (see (2.13) on p. 32) is

$$(\mathbb{X}^\mathsf{T}\hat{\mathbb{W}}\mathbb{X})^{-1} = (\mathbb{X}_R^\mathsf{T}\hat{\mathbb{W}}_R\mathbb{X}_R)^{-1}.$$

It can be easily obtained from the IWLS for either data format.

Deviance

The next thing we need to do is to evaluate the deviance of a logistic model

$$D(\boldsymbol{Y}, \widehat{\boldsymbol{\beta}}) = 2\big[\widetilde{\ell}(\boldsymbol{Y}) - \ell(\widehat{\boldsymbol{\beta}} \mid \boldsymbol{Y})\big],$$

(see Def. 2.7 on p. 30, with dispersion $\varphi = 1$), where $\ell(\widehat{\boldsymbol{\beta}} \mid \boldsymbol{Y})$ is the maximized log-likelihood of our model and $\widetilde{\ell}(\boldsymbol{Y})$ is the maximized log-likelihood of the saturated model.

Let us consider the binomial formulation first. We have K observations with K different values of the covariate vector $\boldsymbol{X}_i$, each observed m_i times, $i = 1, \ldots, K$. The saturated model has K parameters that generate K distinct fitted values $\widetilde{\pi}_i = \frac{Y_i}{m_i}$. The canonical parameter θ_i is $\log\frac{\pi_i}{1-\pi_i}$ and $b(\theta) = \log\frac{1}{1-\pi_i}$. Hence we can write the deviance as

$$\begin{aligned}
D(\boldsymbol{Y}, \widehat{\boldsymbol{\beta}}) &= 2\sum_{i=1}^{K}\sum_{j=1}^{m_i}\left\{Y_{ij}\left(\log\frac{Y_i/m_i}{1-Y_i/m_i} - \log\frac{\widehat{\pi}_i}{1-\widehat{\pi}_i}\right) - \log\frac{1}{1-Y_i/m_i} + \log\frac{1}{1-\widehat{\pi}_i}\right\} \\
&= 2\sum_{i=1}^{K}\left\{Y_i\left(\log\frac{Y_i}{m_i-Y_i} - \log\frac{m_i\widehat{\pi}_i}{m_i-m_i\widehat{\pi}_i}\right) - m_i\left(\log\frac{m_i}{m_i-Y_i} - \log\frac{m_i}{m_i-m_i\widehat{\pi}_i}\right)\right\} \\
&= 2\sum_{i=1}^{K}\left\{Y_i\log\frac{Y_i}{m_i\widehat{\pi}_i} + (m_i-Y_i)\log\frac{m_i-Y_i}{m_i(1-\widehat{\pi}_i)}\right\},
\end{aligned}$$

where the first part of the summand for the i-th group summarizes the successes (the number of successes times the log of the ratio of the observed number of successes divided by the fitted number of successes) and the second part summarizes the failures (the number of failures times the log of the ratio of the observed number of failures divided by the fitted number of failures).

It is important to realize that the deviance can be calculated even if $Y_i = 0$ or $Y_i = m_i$ (then the associated log term that becomes zero is simply omitted).

With the Bernoulli data format, the saturated model has fitted values $\widetilde{\pi}_{ij} = Y_{ij}$ and the deviance becomes (consider the special case of the above with $m_i = 1$)

$$2\sum_{i=1}^{K}\sum_{j=1}^{m_i}\left\{Y_{ij}\log\frac{Y_{ij}}{\widehat{\pi}_i} + (1-Y_{ij})\log\frac{1-Y_{ij}}{1-\widehat{\pi}_i}\right\},$$

which is *different* from the deviance calculated from the binomial data format unless $m_i = 1$ for all i.

Which deviance is the right one? The difference between them stems from the selection of the saturated model. If the data have K distinct values of the covariate vector, the most general model that can be fitted has K distinct fitted values and hence at most K parameters. So, the saturated model that was used to develop the deviance for the Bernoulli data format does not in fact exist. It also follows that the deviance tests that subtract deviances of larger models from deviances of submodels (Theorem 2.9(iii)) are not affected by the form of the deviance (the log-likelihood of the saturated model is canceled) as long as the same saturated model is used in both.

Statistical software will calculate the deviance blindly according to the format the data are entered in (binomial deviance for binomial data format, alternative deviance for Bernoulli data format). Thus, the deviance the software reports for the Bernoulli data format will be wrong but deviance tests of submodels will still be correct.

When all covariates in the dataset are discrete with finite support and data are entered in the binomial data format, K stays constant. Then the saturated model with K parameters satisfies the assumptions of maximum likelihood theory and the binomial deviance $D(\boldsymbol{Y}, \widehat{\boldsymbol{\beta}})$ converges in distribution to χ^2_{K-p} as $m_i \to \infty$ for all i if the current model is valid. Thus, when all m_i are sufficiently large, the deviance can be used as a goodness of fit statistic for deciding whether the current model describes the data sufficiently well (deviance larger than the quantile $\chi^2_{K-p}(1-\alpha)$ indicates that the model does not fit well). However, we must remember that such tests can be done only when all their assumptions are fulfilled:

1. All covariates are discrete
2. There are enough observations in each group
3. The deviance was calculated from the binomial data format

Deviances calculated from the Bernoulli data format cannot ever be used for goodness-of-fit testing but work for submodel testing.

Pearson X^2

The situation with Pearson X^2 statistic is similar. Consider first the Pearson residuals calculated as $\widehat{\mathbb{W}}^{1/2}(\widehat{\boldsymbol{Z}} - \mathbb{X}\widehat{\boldsymbol{\beta}})$ (see Sec. 2.8.1).

Bernoulli data format

With *Bernoulli data format*, the Pearson residuals are

$$r_{ij}^P = \frac{Y_{ij}^* - \widehat{\pi}_i}{\sqrt{\widehat{\pi}_i(1-\widehat{\pi}_i)}}.$$

When $Y_{ij}^* = 1$, the Pearson residual is $\sqrt{\frac{1-\widehat{\pi}_i}{\widehat{\pi}_i}}$. When $Y_{ij}^* = 0$, the Pearson residual is $-\sqrt{\frac{\widehat{\pi}_i}{1-\widehat{\pi}_i}}$. [Think what happens when you plot these residuals against linear predictor or against one of the covariates.]

The Pearson X^2 statistic is obtained by summing squares of Pearson residuals. We get

$$X^2 = \sum_{i=1}^{K}\left[Y_i\frac{1-\widehat{\pi}_i}{\widehat{\pi}_i} + (m_i - Y_i)\frac{\widehat{\pi}_i}{1-\widehat{\pi}_i}\right] = \sum_{i=1}^{K}\left[\frac{Y_i}{m_i\widehat{\pi}_i}m_i(1-\widehat{\pi}_i) + \frac{m_i - Y_i}{m_i(1-\widehat{\pi}_i)}m_i\widehat{\pi}_i\right].$$

For a well-fitting model, $Y_i \approx m_i\widehat{\pi}_i$ and $m_i - Y_i \approx m_i(1-\widehat{\pi}_i)$. Hence,

$$X^2 \approx \sum_{i=1}^{K}\left[m_i(1-\widehat{\pi}_i) + m_i\widehat{\pi}_i\right] = \sum_{i=1}^{K} m_i = N.$$

The Pearson X^2 statistic calculated from the Bernoulli format is about equal to the sample size, if the model fits well. This is not a desirable behavior of a goodness-of-fit statistic.

Binomial data format

Pearson residuals for the *binomial data format* are calculated from the reduced data as $\hat{\mathbb{W}}_R^{1/2}(\widehat{\boldsymbol{Z}}_R - \mathbb{X}_R\widehat{\boldsymbol{\beta}})$. There is one residual for each group $i = 1,\ldots,K$ and

$$r_i^P = \frac{Y_i - m_i\widehat{\pi}_i}{\sqrt{m_i\widehat{\pi}_i(1-\widehat{\pi}_i)}},$$

which is the binomial variable Y_i standardized by subtracting the estimated mean and dividing by its estimated standard deviation. For large m_i, these residuals are approximately standard normal.

The Pearson X^2 statistic for the binomial data format is

$$X^2 = \sum_{i=1}^{K}\frac{(Y_i - m_i\widehat{\pi}_i)^2}{m_i\widehat{\pi}_i(1-\widehat{\pi}_i)} = \sum_{i=1}^{K}\frac{(Y_i - m_i\widehat{\pi}_i)^2}{m_i\widehat{\pi}_i} + \sum_{i=1}^{K}\frac{[(m_i - Y_i) - m_i(1-\widehat{\pi}_i)]^2}{m_i(1-\widehat{\pi}_i)},$$

where we used the equality $\frac{1}{\widehat{\pi}_i(1-\widehat{\pi}_i)} = \frac{1}{\widehat{\pi}_i} + \frac{1}{1-\widehat{\pi}_i}$. This is the chi-square statistic for testing goodness of fit in a $2 \times K$ contingency table with p estimated parameters. In a saturated model with $p = K$, the Pearson X^2 statistic is zero. If the fitted model holds and $m_i \to \infty$ for all i, then $X^2 \xrightarrow{\mathsf{D}} \chi^2_{K-p}$. Thus, when all covariates are discrete and the number of successes and failures is large enough in each group, we can test the validity of the fitted model by

Pearson X^2 statistic calculated from the binomial format (but not by the Pearson X^2 statistic calculated from the Bernoulli format of the same dataset).

Statistical software computes Pearson residuals and Pearson X^2 statistics (and the deviance) from the format in which the data are entered. So, it is the responsibility of the analyst to reshape the data *into the binomial format* if these statistics are important for the analysis. Of course, if there is at least one continuous covariate in the model, the two data formats do not differ from each other (or only negligibly).

Hints on logistic regression practice

For submodel testing, use deviance tests. Do not trust Wald tests of individual coefficients reported in model output, especially not for factor covariates. These tests depend on the parametrization of the factor and may give a misleading impression about the significance of the factor. The recommended way to test model terms in R by deviance tests is

```
drop1(...,test="Chisq")
```

These tests work for both Bernoulli and binomial data formats.

Appropriate transformations of continuous covariates can be deduced, e.g., (i) by factorization of the covariate into subintervals (`cut(x,c(-Inf,x1,x2,...,xm,Inf))`) and evaluating trends in the estimated parameters or (ii) by adding a few different transformations to the linear term and testing their significance. Residual plots can be used, too, but they must be smoothed properly.

A common problem in logistic regression is caused by fitted values converging to zero or one in some subgroup. E.g., if gender is included in the model and all men have response $Y_{ij} = 1$, the MLE of π_i is 1 for all men. This sets the diagonal terms of $\hat{\mathbb{W}}$ to zero and estimated coefficients and their standard errors blow up. So if some of the estimated coefficients are incredibly large in absolute value, and have incredibly large standard errors, or if the IWLS algorithm fails to converge, this is the likely reason. Data subgroups for which no success or no failure are observed must be removed from the data set.

The end of lecture 10 (Apr. 1)

3.2. Analysis of Poisson Count Data

Responses with Poisson distribution are typically counts recording the number of occurrences of some event. When a large number of independent Bernoulli trials are performed, with a small success probability at each trial, the observed total number of successes will approximately follow a Poisson distribution. Poisson responses can also arise by observations of independent Poisson processes evaluated at a fixed time. The primary tool for the analysis of Poisson responses is the loglinear regression model.

3.2.1. Poisson loglinear model

Let $Y_1, \dots, Y_n$ be independent random variables, $Y_i \sim \mathsf{Po}(\lambda_i)$. Let λ_i depend on covariates $\boldsymbol{X}_i$ through the identity $\log \lambda_i = \boldsymbol{X}_i^\mathsf{T} \boldsymbol{\beta}$.

Poisson distribution belongs to the exponential family with $\mu_i = \lambda_i$ and $\mathsf{var}\, Y_i = \lambda_i$. The variance function is $V(\mu) = \mu$, the dispersion parameter is $\varphi = 1$, the canonical parameter is $\theta_i = \log \lambda_i$, $b(\theta_i) = \mathrm{e}^{\theta_i}$. The log link is canonical for Poisson distribution.

We have

$$\mathsf{E}\left[Y_i \,\middle|\, \boldsymbol{X}_i\right] = \mathsf{var}\left[Y_i \,\middle|\, \boldsymbol{X}_i\right] = \lambda_i = \exp\{\boldsymbol{X}_i^\mathsf{T} \boldsymbol{\beta}\}.$$

Interpretation of regression parameters

Let $\boldsymbol{X}^\mathsf{T}\boldsymbol{\beta} = \beta_1 + \beta_2 X_2 + \cdots + \beta_p X_p$. Denote $\lambda_0 = \mathsf{E}\left[Y_i \,\middle|\, X_2 = \cdots = X_p = 0\right]$. Then $\log \lambda_0 = \beta_1$ so e^{β_1} is the expected value of Y_i for an individual with zero values in all covariates.

Now consider two individuals with observed covariates $\boldsymbol{x}^0 = (1, x_2, \dots, x_p)^\mathsf{T}$ and $\boldsymbol{x}^j = \boldsymbol{x}^0 + \boldsymbol{e}_j$ (the j-th covariate is increased by 1, the others are the same). Denote $\lambda_{X0} = \mathsf{E}\left[Y_i \,\middle|\, \boldsymbol{X} = \boldsymbol{x}^0\right]$ and $\lambda_{Xj} = \mathsf{E}\left[Y_i \,\middle|\, \boldsymbol{X} = \boldsymbol{x}^j\right]$. Then

$$\beta_j = \log \frac{\lambda_{Xj}}{\lambda_{X0}} \qquad \text{and} \qquad \mathrm{e}^{\beta_j} = \frac{\lambda_{Xj}}{\lambda_{X0}}.$$

Thus e^{β_j} is the proportional increase in $\mathsf{E}\, Y_i$ per unit difference in the covariate X_j. When $\beta_j = 0$ the ratio of expectations is 1 and the covariate has no effect on the expectation given the other covariates.

Estimation of parameters

The likelihood is

$$L_n(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \prod_{i=1}^{n} \exp\{Y_i \log \lambda_i - \lambda_i - \log(Y_i!)\}$$

and the log-likelihood is

$$\ell_n(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \sum_{i=1}^{n} [Y_i \log \lambda_i - \lambda_i - \log(Y_i!)].$$

By Theorem 2.3, the score statistic with the canonical link is

$$\boldsymbol{U}_n(\boldsymbol{\beta} \mid \boldsymbol{Y}) = \sum_{i=1}^{n} (Y_i - \lambda_i) \boldsymbol{X}_i$$

and $\widehat{\boldsymbol{\beta}}_n$ solves the equations

$$\sum_{i=1}^{n} Y_i \boldsymbol{X}_i = \sum_{i=1}^{n} \widehat{\lambda}_i \boldsymbol{X}_i,$$

where

$$\widehat{\lambda}_i = \exp\{\boldsymbol{X}_i^{\mathsf{T}} \widehat{\boldsymbol{\beta}}_n\}.$$

The MLE of $\boldsymbol{\beta}$ is calculated by the IWLS algorithm

$$\widehat{\boldsymbol{\beta}}_n^{(k+1)} = (\mathbb{X}^{\mathsf{T}} \hat{\mathbb{W}}^{(k)} \mathbb{X})^{-1} (\mathbb{X}^{\mathsf{T}} \hat{\mathbb{W}}^{(k)} \widehat{\boldsymbol{Z}}^{(k)})$$

with

$$\hat{\mathbb{W}}^{(k)} = \operatorname{diag}(\widehat{\lambda}_1^{(k)}, \ldots, \widehat{\lambda}_n^{(k)})$$

and $\widehat{\boldsymbol{Z}}^{(k)} = (\widehat{Z}_1^{(k)}, \ldots, \widehat{Z}_n^{(k)})^{\mathsf{T}}$, where

$$\widehat{Z}_i^{(k)} = \boldsymbol{X}_i^{\mathsf{T}} \widehat{\boldsymbol{\beta}}^{(k)} + \frac{Y_i - \widehat{\lambda}_i^{(k)}}{\widehat{\lambda}_i^{(k)}}.$$

The information matrix is $I(\boldsymbol{\beta}) = \mathsf{E}_{\boldsymbol{X}} \lambda_i \boldsymbol{X}_i^{\otimes 2}$, which can be estimated by

$$\widehat{I}_n = \frac{1}{n} \mathbb{X}^{\mathsf{T}} \hat{\mathbb{W}} \mathbb{X} = \frac{1}{n} \sum_{i=1}^{n} \widehat{\lambda}_i \boldsymbol{X}_i^{\otimes 2}.$$

The estimated variance of $\widehat{\boldsymbol{\beta}}_n$ is $(\mathbb{X}^{\mathsf{T}} \hat{\mathbb{W}} \mathbb{X})^{-1}$.

Deviance

The MLEs of the saturated model parameters are $\widetilde{\lambda}_i = Y_i$ The deviance for loglinear model is

$$D(\boldsymbol{Y} \mid \widehat{\boldsymbol{\beta}}) = 2 \sum_{i=1}^{n} \Big[Y_i \log \frac{Y_i}{\widehat{\lambda}_i} - (Y_i - \widehat{\lambda}_i) \Big]. \tag{3.2}$$

According to Theorem 2.9(iii), the difference in deviances between a submodel and a wider model has a limiting χ^2 distribution if the submodel holds. This is used for loglinear model building.

Pearson X^2

The Pearson residual is

$$r_i^P = \frac{Y_i - \widehat{\lambda}_i}{\sqrt{\widehat{\lambda}_i}},$$

the Pearson X^2 statistic is

$$X^2 = \sum_{i=1}^{n} \frac{(Y_i - \widehat{\lambda}_i)^2}{\widehat{\lambda}_i}. \tag{3.3}$$

Aggregated Poisson responses

What if multiple observations share the same covariate vector? Then they have the same mean and the same fitted value. We can apply an analogue to the binomial data format we considered in logistic regression context and come to very similar conclusions.

Change our notation as follows: let $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_K$ be K distinct values of the covariate vector recorded among the $n \geq K$ observations. Let m_i be the number of observations that share the same covariate vector, so that $\sum_{i=1}^{K} m_i = n$. Change the meaning of Y_i: now, let Y_i be **the sum** of the m_i independent Poisson responses sharing the covariate vector $\boldsymbol{X}_i$. Because the sum of independent Poisson variables is Poisson, we have $Y_i \sim \mathsf{Po}(m_i\lambda_i)$. This distribution is in the exponential family, so all results apply without a change (except writing the mean as $m_i\lambda_i$ at each occurrence).

With the aggregated data format, the responses are $Y_1, \ldots, Y_K$, the regression matrix is $K \times p$, and the weight matrix $\hat{\mathbb{W}}$ is $K \times K$. The data set is written more compactly, especially when all covariates are categorical and $K \ll n$. The IWLS uses

$$\hat{\mathbb{W}} = \operatorname{diag}(m_1\widehat{\lambda}_1, \ldots, m_K\widehat{\lambda}_K)$$

and

$$\widehat{Z}_i = \boldsymbol{X}_i^{\mathsf{T}}\widehat{\boldsymbol{\beta}} + \frac{Y_i - m_i\widehat{\lambda}_i}{m_i\widehat{\lambda}_i}.$$

The MLE of λ_i in the saturated model are $\widetilde{\lambda}_i = \frac{Y_i}{m_i}$. Hence, the aggregated deviance is

$$D(\boldsymbol{Y} \mid \widehat{\boldsymbol{\beta}}) = 2\sum_{i=1}^{K}\Big[Y_i \log\frac{Y_i}{m_i\widehat{\lambda}_i} - (Y_i/m_i - \widehat{\lambda}_i)\Big]. \tag{3.4}$$

This is not the same as the deviance defined by (3.2). When all covariates are categorical, K is finite and $m_i \to \infty$ for all $i = 1, \ldots, K$, then our aggregated deviance (3.4) converges in distribution to χ^2_{K-p} as long as the current model is valid. This is not true for the deviance defined by (3.2). On the other hand, differences in deviances between a submodel and a larger model are always correct no matter if we aggregate the data or not.

The Pearson residual for aggregated Poisson data is

$$r_i^P = \frac{Y_i - m_i\widehat{\lambda}_i}{\sqrt{m_i\widehat{\lambda}_i}}, \quad i = 1, \ldots, K,$$

and the Pearson X^2 statistic is

$$X^2 = \sum_{i=1}^{K}\frac{(Y_i - m_i\widehat{\lambda}_i)^2}{m_i\widehat{\lambda}_i}.$$

This is the χ^2 goodness-of-fit test statistic for multinomial distribution with K outcome levels and p estimated parameters. If all covariates are categorical, K is finite and $m_i \to \infty$ for all $i = 1, \ldots, K$, then the aggregated Pearson X^2 statistic converges in distribution to χ^2_{K-p} as long as the current model is valid.

Pearson X^2 ***statistic*** *can be used for goodness-of-fit testing of models with categorical covariates (in any model, not only logistic or loglinear). The deviance can be used for this purpose as well, and has the same asymptotic distribution. However, only deviance can be used to compare a model with a submodel. Differences in Pearson X^2 statistics do not have asymptotic χ^2 distribution. This is why we prefer deviance tests, while Pearson X^2 tests are considered secondary and of limited importance.*

3.2.2. Modelling Poisson process intensity

So far we considered independent responses Y_i with distribution $\mathsf{Po}(\lambda_i)$ and expressed the effect of covariates on λ_i. However, this assumes that the responses are counts observed over some standardized time interval, e.g., month, week, year — otherwise the means would be affected by the different duration.

Imagine that we want to compare the expected number of traffic accidents caused by men vs. women across different ages. Each observation is one driver and the response is the number of accidents caused by that driver. The covariates are gender and current age. But – for how long are those accidents recorded? Over the whole lifetime? That would induce an artificial age effect, older drivers having more accidents than younger ones. So we would use the number of accidents over the past five years. That would be OK if we remove drivers who have had their driver's licences for less than five years. But they are a particularly interesting subgroup, suspected of causing more accidents than the more experienced drivers. We do not want to exclude them. Also, it is quite possible that men are driving longer trips than women, and younger drivers longer and more frequent trips than elderly drivers: we should take that into account, too. So the best approach would be to standardize the number of accidents for the number of km driven during the last five years and compare the mean number of accidents per 100,000 km driven between men and women, and between different ages. Suppose that we observe the number of km driven over the past 5 years for each participant. How do we perform the analysis?

In general, observations of Poisson counts can be understood as realizations of Poisson processes recorded at some time. A homogeneous Poisson process with intensity λ is a random process $N(t)$, $t \geq 0$, with the following properties:

- $N(0) = 0$;
- N has independent increments, that is for any $t_1 < t_2 < \cdots < t_j$, the random variables $N(t_2) - N(t_1)$, $N(t_3) - N(t_2)$, …, $N(t_j) - N(t_{j-1})$ are independent;

- $N(t) \sim \mathsf{Po}(\lambda t)$.

So, it is a non-decreasing piecewise constant process with values in $\{0, 1, 2, \ldots\}$. It can be shown that the times between successive jumps of $N(t)$ are independent variables with distribution $\mathsf{Exp}(\lambda)$.

Now suppose that we observe iid vectors $(Y_i, t_i, \boldsymbol{X}_i)$, where t_i is the observation time and Y_i is a realization of a Poisson process with intensity λ_i observed at the time t_i. We are interested in estimating the effects of $\boldsymbol{X}_i$ on the intensity λ_i taking into account the observation time t_i.

Note: *The times t_i can be measured on some real time scale (days, months, years,...) but they can also be non-decreasing transformations of time, such as the number of km driven (see the example with traffic accidents), amount of money spent, etc. The times need not even be continuous, discrete time scales are OK, too.*

We have $Y_i \sim \mathsf{Po}(\lambda_i t_i)$, hence $\mathsf{E}\, Y_i = \mathsf{var}\, Y_i = \lambda_i t_i$. The intensity $\lambda_i = \mathsf{E}\, Y_i / t_i$ describes the expected number of events observed during a unit time interval. We use the log link for λ_i: $\log \lambda_i = \boldsymbol{X}_i^\top \boldsymbol{\beta}$, hence $\lambda_i = \mathrm{e}^{\boldsymbol{X}_i^\top \boldsymbol{\beta}}$. It follows that

$$\mathsf{E}\, Y_i = \lambda_i t_i = t_i \mathrm{e}^{\boldsymbol{X}_i^\top \boldsymbol{\beta}} = \mathrm{e}^{\log t_i + \boldsymbol{X}_i^\top \boldsymbol{\beta}}.$$

So, the observation time can be simply taken into account by adding $\log t_i$ to the linear predictor. We can consider it another covariate, with a regression parameter that is *a priori* known to be 1 and hence need not be estimated. Such a term is called *an offset* in GLM terminology. Adding an offset to the linear predictor preserves the structure of the GLM, all formulae and results remain valid without change. In R function `glm()`, an offset term is specified by adding `+offset(var)` to the model formula.

The extension of the Poisson loglinear model to homogeneous Poisson processes is important because it provides a very simple solution to a frequently encountered practical problem. It is very useful to remember this.

The end of lecture 11 (Apr. 8)

3.3. Loglinear Models for Contingency Tables

3.3.1. Two-way contingency table

Consider discrete random variables $X \in \{1, \ldots, I\}$ and $Z \in \{1, \ldots, J\}$. Observe n independent realizations $(X_1, Z_1), \ldots, (X_n, Z_n)$ of this pair. Denote the observed count of the pair $(X = i, Z = j)$ by $n_{ij} = \sum_{l=1}^{n} \mathbb{1}(X_l = i, Z_l = j)$. The observed counts (also called *frequencies*) can be arranged into a two-way contingency table

	$Z=1$	$\cdots$	$Z=J$	Total
$X=1$	n_{11}	$\cdots$	n_{1J}	n_{1+}
$\vdots$	$\vdots$		$\vdots$	$\vdots$
$X=I$	n_{I1}	$\cdots$	n_{IJ}	n_{I+}
Total	n_{+1}	$\cdots$	n_{+J}	$n_{++}=n$

where $n_{i+}=\sum_{j=1}^{J} n_{ij}$ and $n_{+j}=\sum_{i=1}^{I} n_{ij}$.

Denote the expected cell frequencies

$$m_{ij}=\mathsf{E}\, n_{ij}, \qquad m_{i+}=\sum_{j=1}^{J} m_{ij}, \qquad m_{+j}=\sum_{i=1}^{I} m_{ij},$$

and $m_{++}=\sum_{i=1}^{I}\sum_{j=1}^{J} m_{ij}$. The cell probabilities are

$$\pi_{ij}=\mathrm{P}[X=i,Z=j], \qquad \pi_{i+}=\sum_{j=1}^{J}\pi_{ij}=\mathrm{P}[X=i], \qquad \pi_{+j}=\sum_{i=1}^{I}\pi_{ij}=\mathrm{P}[Z=j].$$

Obviously, $\pi_{++}=\sum_{i=1}^{I}\sum_{j=1}^{J}\pi_{ij}=1$.

The cell probabilities can be also arranged into a table:

	$Z=1$	$\cdots$	$Z=J$	Total
$X=1$	π_{11}	$\cdots$	π_{1J}	π_{1+}
$\vdots$	$\vdots$		$\vdots$	$\vdots$
$X=I$	π_{I1}	$\cdots$	π_{IJ}	π_{I+}
Total	π_{+1}	$\cdots$	π_{+J}	$\pi_{++}=1$

The expected frequencies are related to the cell probabilities as follows (we allow n to be random):

$$m_{ij}=\mathsf{E}\, n_{ij}=\mathsf{E}\sum_{l=1}^{n}\mathbb{1}(X_l=i,Z_l=j)=\mathsf{E}\,\mathsf{E}\big[\sum_{l=1}^{n}\mathbb{1}(X_l=i,Z_l=j)\,\big|n\big]=\mathsf{E}\, n\pi_{ij}=m_{++}\pi_{ij},$$

so $\pi_{ij}=m_{ij}/m_{++}$.

The conditional probabilities can be expressed as follows:

$$\mathrm{P}\big(X=i\,\big|Z=j\big)=\frac{\pi_{ij}}{\pi_{+j}}=\frac{m_{ij}}{m_{+j}} \quad \text{and} \quad \mathrm{P}\big(Z=j\,\big|X=i\big)=\frac{\pi_{ij}}{\pi_{i+}}=\frac{m_{ij}}{m_{i+}}.$$

The goal is to use the observed counts n_{ij} to model the cell probabilities π_{ij}, investigate the marginal distributions of X and Z and the associations between X and Z.

3.3.2. Distributions of observed counts

In order to analyze a contingency table by maximum likelihood methods, we have to specify the joint distribution of the observed data, i.e., the counts in the contingency table. There are three reasonable models that arise by different ways of collecting data summarized in the table:

Poisson distribution

Poisson distribution of observed counts arises when the observations (X_i, Z_i) from which the table is built arrive randomly over a given period of time.

For example, we investigate associations between tooth decay ($X = 1$ yes, $X = 2$ no) and soft drink consumption ($Z = 1$ never or rarely, $Z = 2$ sometimes, $Z = 3$ frequently). We include young children (age 6–12) who come to a dentist's office for prevention check-up between January and June of a certain year (if their parents are willing to provide the required information). With this data collection method, the total sample size n is random and the observed cell counts in the resulting table can be assumed to be realizations of independent Poisson processes with different intensity. Then, the whole table can be modelled as independent Poisson variables.

Let $n_{11}, \ldots, n_{IJ}$ be independent random variables with Poisson distributions $n_{ij} \sim \mathsf{Po}(m_{ij})$. It follows $\mathsf{E}\, n_{ij} = \mathsf{var}\, n_{ij} = m_{ij}$. The joint density of the whole table is

$$\mathrm{P}[n_{11} = k_{11}, \ldots, n_{IJ} = k_{IJ}] = \prod_{i,j} \frac{1}{k_{ij}!} m_{ij}^{k_{ij}} \mathrm{e}^{-m_{ij}}, \qquad k_{ij} = 0, 1, 2, \ldots.$$

The total number of observations $n = \sum_{i,j} n_{ij}$ is a random variable with the distribution $\mathsf{Po}(m_{++})$.

The asymptotics does not work by observing an increasing number of independent Poisson variables (the total IJ is fixed) but by letting $m_{++} \to \infty$. The asymptotic MLE theory for iid data does not apply to this case.

Multinomial distribution

Multinomial distribution of observed counts arises when the total number of observations n is fixed in advance.

If, in the previous example, we plan to enroll $n = 100$ children and collect data until the planned sample size is reached, we obviously end up with multinomial distribution for the observed contingency table.

Let the vector $(n_{11}, \ldots, n_{IJ})$ follow the multinomial distribution $\mathsf{Mult}_{IJ}(n, \pi)$, where $\pi = (\pi_{11}, \ldots, \pi_{IJ})^\mathsf{T}$. The joint density of the whole table is

$$\mathsf{P}[n_{11} = k_{11}, \ldots, n_{IJ} = k_{IJ}] = n! \prod_{i,j} \frac{1}{k_{ij}!} \pi_{ij}^{k_{ij}}, \qquad k_{ij} = 0, 1, \ldots, n, \quad \sum_{i,j} k_{ij} = n.$$

The total number of observations n is fixed, $n_{ij} \sim \mathsf{Bi}(n, \pi_{ij})$, $\mathsf{E}\, n_{ij} = n\pi_{ij}$, $\mathsf{var}\, n_{ij} = n\pi_{ij}(1 - \pi_{ij})$, the counts are not independent.

The contingency table can be expressed by summing n iid random vectors, each with distribution $\mathsf{Mult}_{IJ}(1, \pi)$. The asymptotics works through letting $n \to \infty$. The asymptotic MLE theory for iid data applies to this case.

Row multinomial distribution

Row multinomial distribution of observed counts arises when all the row totals n_{i+} are fixed in advance.

We obtain row multinomial distribution if, in the previous example, we plan to enroll $n_{1+} = 50$ children with tooth decay and $n_{2+} = 50$ children without tooth decay and collect data until the planned sample size is reached in both subgroups.

Let the vectors $(n_{i1}, \ldots, n_{iJ})$, $i = 1, \ldots, I$, be independent with the multinomial distribution $\mathsf{Mult}_J(n_{i+}, \pi_i)$, where $\pi_i = (\pi_{i1}/\pi_{i+}, \ldots, \pi_{iJ}/\pi_{i+})^\mathsf{T}$. The joint density of the whole table is

$$\mathsf{P}[n_{11} = k_{11}, \ldots, n_{IJ} = k_{IJ}] = \prod_i n_{i+}! \prod_j \frac{1}{k_{ij}!} \left(\frac{\pi_{ij}}{\pi_{i+}} \right)^{k_{ij}}, \quad k_{ij} = 0, 1, \ldots, n, \; \sum_j k_{ij} = n_{i+}.$$

The numbers of observations n_{i+} in the I rows of the table are fixed, $n_{ij} \sim \mathsf{Bi}(n_{i+}, \frac{\pi_{ij}}{\pi_{i+}})$, $\mathsf{E}\, n_{ij} = n_{i+} \frac{\pi_{ij}}{\pi_{i+}}$, $\mathsf{var}\, n_{ij} = n_{i+} \frac{\pi_{ij}}{\pi_{i+}} (1 - \frac{\pi_{ij}}{\pi_{i+}})$, the counts are independent between rows but dependent within rows.

The asymptotics works through letting $n_{i+} \to \infty$ for all i at the same rate. The asymptotic MLE theory for iid data applies to this case.

Of course, we could consider column multinomial distribution as well, but it is just a transposition of the row multinomial case.

Equivalence of Poisson and multinomial models

We start with a result stating that Poisson and multinomial distributions are related through conditioning on the total count.

Lemma 3.1. *Let $X_i \sim Po(\lambda_i)$ be independent random variables, $i = 1,\dots,n$. Then the conditional joint distribution of the random vector $(X_1,\dots,X_n)^T$ given $\sum_{i=1}^n X_i = s$ is $Mult_n(s,\boldsymbol{p})$, where $\boldsymbol{p} = (p_1,\dots,p_n)^T$ and $p_i = \lambda_i / \sum_{j=1}^n \lambda_j$.* ♢

Proof. Calculate the conditional probability

$$\mathrm{P}\big(X_1 = k_1,\dots,X_n = k_n \,\big|\, \sum_{i=1}^n X_i = s\big) = \frac{\mathrm{P}\left[X_1 = k_1,\dots,X_n = k_n, \sum_{i=1}^n X_i = s\right]}{\mathrm{P}\left[\sum_{i=1}^n X_i = s\right]}. \qquad (*)$$

The probability in the numerator is zero unless $\sum_{i=1}^n k_i = s$; in that case the event $\sum_{i=1}^n X_i = s$ can be dropped and we have an intersection of independent events. The probability in the denominator is determined from the known result about summing independent Poisson variables $\sum_{i=1}^n X_i \sim \mathsf{Po}(\sum_{i=1}^n \lambda_i)$. Hence

$$(*) = \frac{\prod_{i=1}^n \lambda_i^{k_i} \mathrm{e}^{-\lambda_i} \frac{1}{k_i!}}{\big(\sum_i \lambda_i\big)^s \mathrm{e}^{-\sum_i \lambda_i} \frac{1}{s!}} = \frac{s!}{k_1!\cdots k_n!} \frac{\lambda_1^{k_1}\cdots\lambda_n^{k_n}}{\big(\sum_i \lambda_i\big)^{k_1}\cdots\big(\sum_i \lambda_i\big)^{k_n}} = \frac{s!}{k_1!\cdots k_n!}\, \pi_1^{k_1}\cdots\pi_n^{k_n}$$

with $\pi_i = \frac{\lambda_i}{\sum_i \lambda_i}$. The proof is completed. □

Corollary. Let $n_{ij} \sim \mathsf{Po}(m_{ij})$ be independent, $i = 1,\dots,I$, $j = 1,\dots,J$. Then:

- The conditional joint distribution of $(n_{11},\dots,n_{IJ})^\mathsf{T}$ given $n_{++} = n$ is $\mathsf{Mult}_{IJ}(n,\boldsymbol{\pi})$, where the components of $\boldsymbol{\pi}$ are $\pi_{ij} = m_{ij}/m_{++}$ ($\Rightarrow$ *multinomial distribution*).
- The conditional joint distribution of $(n_{i1},\dots,n_{iJ})^\mathsf{T}$ given n_{i+} is $\mathsf{Mult}_J(n_{i+},\boldsymbol{\pi}_i)$, where the components of $\boldsymbol{\pi}_i$ are $\pi_{ij} = m_{ij}/m_{i+} = \pi_{ij}/\pi_{i+}$ ($\Rightarrow$ *row multinomial distribution*).

The corollary states that both multinomial and row multinomial distributions of a contingency table can be obtained from Poisson distribution by conditioning on some observed totals.

Assume that the loglinear model holds for the expected frequencies m_{ij}, in particular,

$$\log \mathsf{E}\, n_{ij} = \alpha + \boldsymbol{\beta}^\mathsf{T}\boldsymbol{X}_{ij} \quad \text{or} \quad m_{ij} = \mathrm{e}^{\alpha+\boldsymbol{\beta}^\mathsf{T}\boldsymbol{X}_{ij}},$$

where α is the intercept and $\boldsymbol{X}_{ij}$ is a vector of covariates characterizing the (i,j)-th cell. The maximum dimension of $\boldsymbol{X}_{ij}$ is $IJ-1$. The cell probabilities π_{ij} can be expressed as follows:

$$\pi_{ij} = \frac{m_{ij}}{m_{++}} = \frac{\mathrm{e}^{\boldsymbol{\beta}^\mathsf{T}\boldsymbol{X}_{ij}}}{\sum_{k,l} \mathrm{e}^{\boldsymbol{\beta}^\mathsf{T}\boldsymbol{X}_{kl}}}. \qquad (3.5)$$

Theorem 3.2. *The likelihood functions for estimation of parameters $\boldsymbol{\beta}$ in the loglinear model $\log m_{ij} = \alpha + \boldsymbol{\beta}^T\boldsymbol{X}_{ij}$ arising from Poisson or multinomial sampling distributions are equivalent (they differ only by a multiplicative constant that does not depend on $\boldsymbol{\beta}$).* ♢

Note. Theorem 3.2 does not deal with estimation of the intercept α – in fact, the intercept is not even identifiable in the multinomial model. This is obvious from expression (3.5).

Proof. First, write the Poisson likelihood for the loglinear model $\log m_{ij} = \alpha + \boldsymbol{\beta}^\top \boldsymbol{X}_{ij}$ with data $\boldsymbol{n} = (n_{11}, \ldots, n_{IJ})^\top$.

$$L_P(\alpha, \boldsymbol{\beta} \mid \boldsymbol{n}) = \prod_{i,j} \frac{1}{n_{ij}!} m_{ij}^{n_{ij}} \mathrm{e}^{-mij}$$

and express the log-likelihood as

$$\ell_p(\alpha, \boldsymbol{\beta}) = \sum_{i,j} n_{ij} \log m_{ij} - m_{++} - \underbrace{\sum_{i,j} \log n_{ij}!}_{\equiv c_P},$$

where the constant c_P can be ignored.

Next, write the multinomial likelihood. When we express cell probabilities in terms of the expected frequencies using the loglinear model, we get

$$\pi_{ij} = \frac{m_{ij}}{m_{++}} = \frac{\mathrm{e}^{\alpha + \boldsymbol{\beta}^\top \boldsymbol{X}_{ij}}}{\sum_{i,j} \mathrm{e}^{\alpha + \boldsymbol{\beta}^\top \boldsymbol{X}_{ij}}} = \frac{\mathrm{e}^{\boldsymbol{\beta}^\top \boldsymbol{X}_{ij}}}{\sum_{i,j} \mathrm{e}^{\boldsymbol{\beta}^\top \boldsymbol{X}_{ij}}}. \tag{3.6}$$

The parameter α dropped out, the multinomial likelihood is only a function of $\boldsymbol{\beta}$. Hence

$$L_M(\boldsymbol{\beta} \mid \boldsymbol{n}) = n! \prod_{i,j} \frac{1}{n_{ij}!} \left(\frac{m_{ij}}{m_{++}} \right)^{n_{ij}}$$

and the log-likelihood is

$$\ell_M(\boldsymbol{\beta}) = \sum_{i,j} n_{ij} \log m_{ij} - n \log m_{++} + \underbrace{\log \frac{n!}{n_{11}! \cdots n_{IJ}!}}_{\equiv c_M}.$$

Now go back to the Poisson log-likelihood ℓ_p and reparametrize it as a function of parameters $(m_{++}, \boldsymbol{\beta})$ instead of $(\alpha, \boldsymbol{\beta})$ – this is a one-to-one transformation of parameters. The Poisson log-likelihood can be written as

$$\ell_p(m_{++}, \boldsymbol{\beta}) = \underbrace{\sum_{i,j} n_{ij} \log m_{ij} - n \log m_{++}}_{= \ell_M(\boldsymbol{\beta}) - c_M} + \underbrace{n \log m_{++} - m_{++}}_{\text{denote } \ell^*(m_{++})} - c_p.$$

The first part is the multinomial log-likelihood (the conditional log-likelihood given the total size n) without its irrelevant constant, the second part is the marginal log-likelihood for the sample size $n \sim \mathsf{Po}(m_{++})$. The first part depends only on $\boldsymbol{\beta}$ but not on α or m_{++}, the second part depends on m_{++} but not on $\boldsymbol{\beta}$.

Thus, in both Poisson and multinomial models, the MLE of the parameters $\boldsymbol{\beta}$ are obtained by maximizing the same function

$$\begin{aligned}\sum_{i,j} n_{ij}\log m_{ij} - n\log m_{++} &= \sum_{i,j} n_{ij}(\alpha+\boldsymbol{\beta}^\top \boldsymbol{X}_{ij}) - n\log\sum_{i,j}\mathrm{e}^{\alpha+\boldsymbol{\beta}^\top \boldsymbol{X}_{ij}}\\ &= \sum_{i,j} n_{ij}\boldsymbol{\beta}^\top \boldsymbol{X}_{ij} + n\alpha - n\log\mathrm{e}^{\alpha} - n\log\sum_{i,j}\mathrm{e}^{\boldsymbol{\beta}^\top \boldsymbol{X}_{ij}}\\ &= \sum_{i,j} n_{ij}\boldsymbol{\beta}^\top \boldsymbol{X}_{ij} - n\log\sum_{i,j}\mathrm{e}^{\boldsymbol{\beta}^\top \boldsymbol{X}_{ij}}\end{aligned}$$

over $\boldsymbol{\beta}$. The likelihoods of both models are equivalent as far as estimation of $\boldsymbol{\beta}$ is concerned. □

Theorem 3.2 can be extended to row multinomial distribution as follows:

Theorem 3.3. *(Palmgren 1981) The likelihood functions for estimation of parameters $\boldsymbol{\beta}$ in the loglinear model $\log m_{ij} = \alpha_i + \boldsymbol{\beta}^T \boldsymbol{X}_{ij}$ arising from Poisson or row-multinomial sampling distributions are equivalent (they differ only by a multiplicative constant that does not depend on $\boldsymbol{\beta}$).* ♢

Note. Row multinomial sampling requires row-specific intercept in the loglinear model.

Corollary. Expressions for any quantity derived from the likelihood function for $\boldsymbol{\beta}$ (score function, information matrix, the MLE) and their properties (asymptotic distributions, test statistics, confidence intervals) are the same no matter which of the three distributions generated the contingency table.

When the data are generated by the Poisson model, they can be transformed to the multinomial model by conditioning on the observed cell count total $n = n_{++}$. The asymptotic results hold in the multinomial model (the data are equivalent to n independent observations from Mult_1). The formulae can be derived from the theory of GLM for the loglinear model with Poisson distribution.

In the rest of this section we assume the loglinear model with Poisson distribution but the results apply to multinomial models without change.

The end of lecture 12 (Apr. 8)

A. Appendix: Maximum Likelihood Theory

A.1. Definition

Consider a random sample $\boldsymbol{X} = (X_1, \ldots, X_n)$ of independent identically distributed random variables (or vectors), each with density $f(x|\boldsymbol{\theta}_X)$ with respect to a σ-finite measure μ. We assume that $f(x|\boldsymbol{\theta}_X) \in \mathscr{F}$, where

$$\mathscr{F} = \{\text{distributions with density } f(x|\boldsymbol{\theta}),\ \boldsymbol{\theta} \in \Theta \subseteq \mathbb{R}^d\}$$

represents a parametric model for the distribution of the data.

The model $\mathscr{F}$ must satisfy the model identifiability condition: For any $\boldsymbol{\theta}_1 \neq \boldsymbol{\theta}_2$ it holds $f(x|\boldsymbol{\theta}_1) \neq f(x|\boldsymbol{\theta}_2)$. In other words, no distribution can be parametrized by several different parameter vectors.

Because of independence, the joint denstity of the random sample $X_1, \ldots, X_n$ is $\prod_{i=1}^n f(x_i|\boldsymbol{\theta}_X)$. The maximum likelihood estimator $\widehat{\boldsymbol{\theta}}$ of the parameter $\boldsymbol{\theta}_X$ is the point from Θ that maximizes the joint density evaluated at the observed values of $X_1, \ldots, X_n$.

Definition A.1 (likelihood, log-likelihood).

- The random function
$$L_n(\boldsymbol{\theta}) \stackrel{\text{df}}{=} \prod_{i=1}^n f(X_i|\boldsymbol{\theta})$$
is called *the likelihood function* for the parameter $\boldsymbol{\theta}$ in the model $\mathscr{F}$.
- The random function
$$\ell_n(\boldsymbol{\theta}) \stackrel{\text{df}}{=} \log L_n(\boldsymbol{\theta}) = \sum_{i=1}^n \log f(X_i|\boldsymbol{\theta})$$
is called *the log-likelihood function*. ▽

Definition A.2 (maximum likelihood estimator). *The maximum likelihood estimator* (MLE) of the parameter $\boldsymbol{\theta}_X$ in the model $\mathscr{F}$ is defined as

$$\widehat{\boldsymbol{\theta}}_n = \arg\max_{\boldsymbol{\theta} \in \Theta} L_n(\boldsymbol{\theta}).$$ ▽

Note. Since the logarithm is strictly increasing, $L_n(\boldsymbol{\theta})$ and $\ell_n(\boldsymbol{\theta})$ attain the maximum at the same point.

Definition A.3. Let P and Q be probability measures on the same probability space with densities p and q with respect to the same σ-finite measure μ (for example, $\mu = P + Q$). Define

$$K(P,Q) = \begin{cases} \mathsf{E}_P \log \frac{p(X)}{q(X)} = \int_{\{x:p(x)>0\}} \log \frac{p(x)}{q(x)} p(x)\, d\mu(x) & \text{if } \mathrm{P}[q(X)=0]=0 \\ +\infty & \text{otherwise.} \end{cases}$$

$K(P,Q)$ is called the *Kullback-Leibler distance (divergence)*. ∇

Note. In fact, $K(P,Q)$ is a pseudo-distance: it holds $K(P,Q) \geq 0$, and $K(P,Q) = 0$ if and only if $P = Q$, but it is not symmetric: $K(P,Q) \neq K(Q,P)$.

Theorem A.1. *Suppose the support set $S = \{x \in \mathbb{R} : f(x|\boldsymbol{\theta}) > 0\}$ does not depend on the parameter $\boldsymbol{\theta}$. Denote P_X the induced probability measure of the random variable X_i and P_θ the probability measure associated with the density $f(x|\boldsymbol{\theta})$. Then for any $\boldsymbol{\theta} \neq \boldsymbol{\theta}_X$*

$$\frac{1}{n} \log \frac{L_n(\boldsymbol{\theta}_X)}{L_n(\boldsymbol{\theta})} = \frac{1}{n} \sum_{i=1}^{n} \log \frac{f(X_i|\boldsymbol{\theta}_X)}{f(X_i|\boldsymbol{\theta})} \to K(P_X, P_\theta) \quad P_X - \textit{ almost surely,}$$

and hence

$$\mathrm{P}[\ell_n(\boldsymbol{\theta}_X) > \ell_n(\boldsymbol{\theta})] \to 1 \quad \textit{as } n \to \infty. \qquad \diamondsuit$$

Note. When the number of observations increases to infinity, the (log-)likelihood function at the true parameter will be with a large probability larger than the (log-)likelihood function at any other parameter. This observation justifies the idea of estimating the parameters by maximizing the log-likelihood over all possible parameter vectors.

A.2. The calculation of the maximum likelihood estimator

The maximum likelihood estimator is usually determined by differentiation of the log-likelihood. The first derivative is set to zero and it is verified that the second derivative is negative definite.

Definition A.4 (score, information).

- The random vector
$$\boldsymbol{U}(\boldsymbol{\theta}|X_i) \stackrel{\mathrm{df}}{=} \frac{\partial}{\partial \boldsymbol{\theta}} \log f(X_i|\boldsymbol{\theta})$$
is called *the score function* for the parameter $\boldsymbol{\theta}$ in the model $\mathscr{F}$.

- The random vector
$$\boldsymbol{U}_n(\boldsymbol{\theta}|\boldsymbol{X}) \stackrel{\text{df}}{=} \sum_{i=1}^{n} \boldsymbol{U}(\boldsymbol{\theta}|X_i) = \sum_{i=1}^{n} \frac{\partial}{\partial \boldsymbol{\theta}} \log f(X_i|\boldsymbol{\theta})$$
is called *the score statistic*.
- The random matrix
$$I(\boldsymbol{\theta}|X_i) \stackrel{\text{df}}{=} -\frac{\partial}{\partial \boldsymbol{\theta}^{\mathsf{T}}} \boldsymbol{U}(\boldsymbol{\theta}|X_i) = -\frac{\partial^2}{\partial \boldsymbol{\theta}\, \partial \boldsymbol{\theta}^{\mathsf{T}}} \log f(X_i|\boldsymbol{\theta})$$
is called the contribution of the i-th observation to the information matrix.
- The random matrix
$$I_n(\boldsymbol{\theta}|\boldsymbol{X}) \stackrel{\text{df}}{=} -\frac{1}{n} \frac{\partial}{\partial \boldsymbol{\theta}^{\mathsf{T}}} \boldsymbol{U}_n(\boldsymbol{\theta}|\boldsymbol{X}) = \frac{1}{n} \sum_{i=1}^{n} I(\boldsymbol{\theta}|X_i)$$
is called *the observed information matrix*.
- The matrix
$$I(\boldsymbol{\theta}) \stackrel{\text{df}}{=} \mathsf{E}\, I(\boldsymbol{\theta}|X_i) = -\mathsf{E}\, \frac{\partial^2}{\partial \boldsymbol{\theta}\, \partial \boldsymbol{\theta}^{\mathsf{T}}} \log f(X_i|\boldsymbol{\theta})$$
is called *the expected (Fisher) information matrix*. ∇

If the set Θ is open, the MLE $\widehat{\boldsymbol{\theta}}_n$ solves the system of equations $\boldsymbol{U}_n(\widehat{\boldsymbol{\theta}}_n|\boldsymbol{X}) = \mathbf{0}$, that is
$$\sum_{i=1}^{n} \frac{\partial}{\partial \boldsymbol{\theta}} \log f(X_i|\widehat{\boldsymbol{\theta}}_n) = \mathbf{0}.$$
This system is called the *likelihood equations*.

The solution to the likelihood equations need not exist. Sometimes there may be multiple solutions, at most one of which is the MLE. If $I_n(\widehat{\boldsymbol{\theta}}_n|\boldsymbol{X}) > 0$ (the observed information is positive definite at $\widehat{\boldsymbol{\theta}}_n$), we know that $\widehat{\boldsymbol{\theta}}_n$ is at least a local maximum. If $I_n(\boldsymbol{\theta}|\boldsymbol{X}) > 0$ for every $\boldsymbol{\theta} \in \Theta$, the log-likelihood function is concave and the solution to the likelihood equations must be the global maximum and hence the MLE.

In most cases no explicit solution can be found and the MLE must be calculated by numerical methods. There are two commonly used numerical methods for solving the likelihood equations. Let $\widehat{\boldsymbol{\theta}}^{(r)}$ be the r-th iteration to the solution.

- **The Newton-Raphson method:** $\widehat{\boldsymbol{\theta}}^{(r+1)} = \widehat{\boldsymbol{\theta}}^{(r)} + [nI_n(\widehat{\boldsymbol{\theta}}^{(r)}|\boldsymbol{X})]^{-1} \boldsymbol{U}_n(\widehat{\boldsymbol{\theta}}^{(r)}|\boldsymbol{X})$
- **The Fisher Scoring method:** $\widehat{\boldsymbol{\theta}}^{(r+1)} = \widehat{\boldsymbol{\theta}}^{(r)} + [nI(\widehat{\boldsymbol{\theta}}^{(r)})]^{-1} \boldsymbol{U}_n(\widehat{\boldsymbol{\theta}}^{(r)}|\boldsymbol{X})$

They are iterated until the change in $\widehat{\boldsymbol{\theta}}$ from one iteration to the next is sufficiently small or until $\boldsymbol{U}_n(\widehat{\boldsymbol{\theta}})$ is sufficiently close to $\mathbf{0}$. The only difference between the two methods is in the information matrix: N-R uses the observed information, FS uses the expected information.

Both require setting $\widehat{\boldsymbol{\theta}}^{(1)}$, the starting value for numerical approximation, and are sensitive to its choice.

A.3. Properties of the maximum likelihood estimator

Maximum likelihood estimators are consistent and asymptotically normal as long as so called *regularity conditions* are satisfied.

Conditions (Regularity conditions for maximum likelihood estimators).

R1. The number of parameters d in the model $\mathscr{F}$ is constant.

R2. The support set $S = \{x \in \mathbb{R} : f(x|\boldsymbol{\theta}) > 0\}$ does not depend on the parameter $\boldsymbol{\theta}$.

R3. The parameter space Θ is an open set.

R4. The density $f(x|\boldsymbol{\theta})$ is sufficiently smooth function of $\boldsymbol{\theta}$ (at least twice continuously differentiable).

R5. The Fisher information matrix $I(\boldsymbol{\theta})$ is finite, regular, and positive definite in a neighborhood of $\boldsymbol{\theta}_X$.

R6. The order of differentiation and integration can be interchanged in expressions such as

$$\frac{\partial}{\partial \boldsymbol{\theta}} \int h(x, \boldsymbol{\theta})\, d\mu(x) = \int \frac{\partial}{\partial \boldsymbol{\theta}} h(x, \boldsymbol{\theta})\, d\mu(x),$$

where $h(x, \boldsymbol{\theta})$ is either $f(x|\boldsymbol{\theta})$ or $\partial f(x|\boldsymbol{\theta})/\partial \boldsymbol{\theta}$.

Note. Take the identity

$$\int_{-\infty}^{\infty} f(x|\boldsymbol{\theta})\, d\mu(x) = 1$$

and differentiate both sides of the equation twice with respect to $\boldsymbol{\theta}$. Regularity condition R6 implies

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial \boldsymbol{\theta}} f(x|\boldsymbol{\theta})\, d\mu(x) = \int_{-\infty}^{\infty} \frac{\partial^2}{\partial \boldsymbol{\theta}\, \partial \boldsymbol{\theta}^{\mathsf{T}}} f(x|\boldsymbol{\theta})\, d\mu(x) = \mathbf{0}. \tag{A.1}$$

Theorem A.2 (consistency of the MLE). *Let conditions R1–R6 hold. Then there exists n_0 and a sequence $\widehat{\boldsymbol{\theta}}_n$ ($n \geq n_0$) of solutions to the likelihood equations $\boldsymbol{U}_n(\widehat{\boldsymbol{\theta}}_n|\boldsymbol{X}) = \mathbf{0}$ such that $\widehat{\boldsymbol{\theta}}_n \xrightarrow{P} \boldsymbol{\theta}_X$.* ♢

Note. If the log-likelihood is strictly concave, the likelihood equations have a unique solution, which is the MLE. It converges in probability to the true parameter. If the log-likelihood is not strictly concave, the likelihood equations may have multiple solutions representing local maxima and minima of the log-likelihood. There is one solution among them (the closest to $\boldsymbol{\theta}_X$), which provides a consistence sequence of estimators. Other solutions may not be close to $\boldsymbol{\theta}_X$ and may not converge to it.

Note. If there exists a sequence $\widetilde{\boldsymbol{\theta}}_n$ of other estimators that are guaranteed to be consistent (for example, moment estimators of $\boldsymbol{\theta}_X$), a consistent MLE can be obtained by taking the root of the likelihood equations, which is closest to $\widetilde{\boldsymbol{\theta}}_n$. Alternatively, one can perform one step of the Newton-Raphson algorithm with $\widetilde{\boldsymbol{\theta}}_n$ as the starting value.

Theorem A.3 (Score function properties). *Let conditions R1–R6 hold. Then*

(i) $E\,\boldsymbol{U}(\boldsymbol{\theta}_X|X_i) = 0$, $var\,\boldsymbol{U}(\boldsymbol{\theta}_X|X_i) = I(\boldsymbol{\theta}_X)$.

(ii) $\frac{1}{\sqrt{n}}\boldsymbol{U}_n(\boldsymbol{\theta}_X|\boldsymbol{X}) \xrightarrow{D} N_d(\mathbf{0}, I(\boldsymbol{\theta}_X))$. ♢

Note. The Fisher information matrix at $\boldsymbol{\theta}_X$ can be calculated in two different ways: from Definition A.4 (the expectation of minus the second derivative of the log density) or from Theorem A.3 (the score function variance).

Theorem A.4 (asymptotic normality of the MLE). *Suppose conditions R1–R6 hold. Let* $\widehat{\boldsymbol{\theta}}_n$ *be a consistent sequence of solutions to the likelihood equations. Then*

$$\sqrt{n}(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_X) \xrightarrow{D} N_d(\mathbf{0}, I^{-1}(\boldsymbol{\theta}_X)).$$ ♢

Note.

- The asymptotic variance of the MLE is equal to the inverse of the Fisher information. More information means better precision for estimation.
- The asymptotic variance of the MLE is in a certain sense optimal. Other estimators (e.g., moment estimators) cannot have a smaller asymptotic variance.

Theorem A.5 (asymptotic distribution of the likelihood ratio). *Suppose conditions R1–R6 hold. Let* $\widehat{\boldsymbol{\theta}}_n$ *be a consistent sequence of solutions to the likelihood equations. Then*

$$2\log\frac{L_n(\widehat{\boldsymbol{\theta}}_n)}{L_n(\boldsymbol{\theta}_X)} = 2(\ell_n(\widehat{\boldsymbol{\theta}}_n) - \ell_n(\boldsymbol{\theta}_X)) \xrightarrow{D} \chi^2_d.$$ ♢

Theorem A.6 (the Δ method for the MLE). *Suppose conditions R1–R6 hold. Let* $\widehat{\boldsymbol{\theta}}_n$ *be a consistent sequence of solutions to the likelihood equations. Take* $q : \Theta \to \mathbb{R}^k$ *a continuously differentiable function. Denote* $\boldsymbol{\nu}_X = q(\boldsymbol{\theta}_X)$ *a* $D(\boldsymbol{\theta}) = \partial q(\boldsymbol{\theta})/\partial\boldsymbol{\theta}$. *Then* $\widehat{\boldsymbol{\nu}}_n = q(\widehat{\boldsymbol{\theta}}_n)$ *is the MLE of the parameter* $\boldsymbol{\nu}_X$ *and*

$$\sqrt{n}(\widehat{\boldsymbol{\nu}}_n - \boldsymbol{\nu}_X) \xrightarrow{D} N_k(\mathbf{0}, D(\boldsymbol{\theta}_X)I^{-1}(\boldsymbol{\theta}_X)D(\boldsymbol{\theta}_X)^T).$$ ♢

A.4. Tests based on maximum likelihood theory

The theory of the MLE can be used to derive tests of simple and composite hypotheses about the parameter $\boldsymbol{\theta}_X$.

A.4.1. Testing of simple hypotheses

We want to test the null hypothesis $H_0 : \boldsymbol{\theta}_X = \boldsymbol{\theta}_0$ against the alternative $H_1 : \boldsymbol{\theta}_X \neq \boldsymbol{\theta}_0$, where $\boldsymbol{\theta}_0 \in \Theta$. It is a simple hypothesis because there is just a single distribution in the model $\mathscr{F}$ with the density $f(x|\boldsymbol{\theta}_0)$.

We will introduce three different test statistics for testing H_0.

Definition A.5.

(i) The statistic
$$\lambda_n = \frac{L_n(\widehat{\boldsymbol{\theta}}_n)}{L_n(\boldsymbol{\theta}_0)}$$
is called *the likelihood ratio*.

(ii) The statistic
$$W_n = n(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_0)^{\mathsf{T}} \widehat{I}_n(\widehat{\boldsymbol{\theta}}_n)(\widehat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_0)$$
is called *the Wald statistic*.

(iii) The statistic
$$R_n = \frac{1}{n} \boldsymbol{U}_n(\boldsymbol{\theta}_0|\boldsymbol{X})^{\mathsf{T}} \widehat{I}_n^{-1}(\boldsymbol{\theta}_0) \boldsymbol{U}_n(\boldsymbol{\theta}_0|\boldsymbol{X})$$
is called *the Rao (score) statistic*. ∇

Note. The symbol $\widehat{I}_n$ denotes any consistent estimator of the Fisher information matrix. Three different estimators can be used in Wald and Rao statistics:

1. $\widehat{I}_n(\boldsymbol{\theta}) = I_n(\boldsymbol{\theta}|\boldsymbol{X}) = -\frac{1}{n} \sum_{i=1}^n \frac{\partial^2}{\partial \boldsymbol{\theta}\, \partial \boldsymbol{\theta}^{\mathsf{T}}} \log f(\boldsymbol{\theta}|X_i)$ (the observed information matrix)
2. $\widehat{I}_n(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n \boldsymbol{U}(\boldsymbol{\theta}|X_i)^{\otimes 2}$ (the empirical variance of the score function)
3. $\widehat{I}_n(\boldsymbol{\theta}) = I(\boldsymbol{\theta})$ (the Fisher information matrix)

The most common choice for the Wald statistic is $\widehat{I}_n(\widehat{\boldsymbol{\theta}}_n) = I_n(\widehat{\boldsymbol{\theta}}_n|\boldsymbol{X})$. The most common choice for the Rao statistic is $\widehat{I}_n(\boldsymbol{\theta}_0) = \frac{1}{n} \sum_{i=1}^n \boldsymbol{U}(\boldsymbol{\theta}_0|X_i)^{\otimes 2}$.

Note.

- The likelihood ratio requires the calculation of $\widehat{\boldsymbol{\theta}}_n$ and L_n or ℓ_n. It does not require the calculation of $\boldsymbol{U}_n$ and $\widehat{I}_n$.
- The Wald statistic requires the calculation of $\widehat{\boldsymbol{\theta}}_n$ and $\widehat{I}_n$. It does not require the calculation of L_n and $\boldsymbol{U}_n$.
- Rao statistic requires the calculation of $\boldsymbol{U}_n$ a $\widehat{I}_n$. It does not require the calculation of $\widehat{\boldsymbol{\theta}}_n$ and L_n.

Note. If $d = 1$ (one parameter) and $\theta_0 = 0$, then the Wald statistic can be written as
$$W_n = \left[\frac{\widehat{\theta}_n}{\sqrt{n^{-1} \widehat{I}_n^{-1}(\widehat{\theta}_n)}} \right]^2,$$

where $n^{-1}\widehat{I}_n^{-1}(\widehat{\theta}_n)$ is the estimator of the asymptotic variance of $\widehat{\theta}_n$.

Theorem A.7. *Suppose conditions R1–R6 are satisfied. Let the hypothesis $H_0 : \boldsymbol{\theta}_X = \boldsymbol{\theta}_0$ hold. Then:*

(i)

$$2\log\lambda_n = 2(\ell_n(\widehat{\boldsymbol{\theta}}_n) - \ell_n(\boldsymbol{\theta}_0)) \xrightarrow{D} \chi^2_d$$

(ii)

$$W_n \xrightarrow{D} \chi^2_d$$

(iii)

$$R_n \xrightarrow{D} \chi^2_d \qquad \diamondsuit$$

Note. If H_0 holds, $\widehat{\boldsymbol{\theta}}_n$ should be close to $\boldsymbol{\theta}_0$, $L_n(\widehat{\boldsymbol{\theta}}_n)$ should be close to $L_n(\boldsymbol{\theta}_0)$, and $\boldsymbol{U}_n(\boldsymbol{\theta}_0|\boldsymbol{X})$ should be close to $\mathbf{0}$. Under H_0, all three test statistics have values close to 0. Their large values testify against H_0.

Corollary. Denote by $\chi^2_d(1-\alpha)$ the $(1-\alpha)$-quantile of χ^2_d distribution. Consider tests of $H_0 : \boldsymbol{\theta}_X = \boldsymbol{\theta}_0$ against $H_1 : \boldsymbol{\theta}_X \neq \boldsymbol{\theta}_0$ defined by the rule: reject H_0 in favor of H_1, if

(i) $2\log\lambda_n \geq \chi^2_d(1-\alpha)$ *(likelihood ratio test)*
(ii) $W_n \geq \chi^2_d(1-\alpha)$ *(Wald test)*
(iii) $R_n \geq \chi^2_d(1-\alpha)$ *(score test)*

Each of these tests has asymptotically (for $n \to \infty$) the level α.

Note. It can be shown that these three tests are asymptotically equivalent. For large sample sizes, their results are almost identical. With smaller sample sizes, their results can differ. Investigations of small sample behavior of these test statistics revealed that the likelihood ratio test has the best properties, the Wald test is the worst of the three.

Thus, in practical applications, the likelihood ratio test should be preferred.

Note. Under normality, the three test statistics are identical.

A.4.2. Estimation in the presence of nuisance parameters and testing of composite hypotheses

It is frequently desirable to estimate and test just a small number of parameters in a model that contains a much larger number of parameters. We divide the parameter vector into two subsets: the parameters of interest and the other paramaters – *nuisance parameters*.

Let $\boldsymbol{\theta}$ be divided into $\boldsymbol{\theta}_A$ containing the first m components of $\boldsymbol{\theta}$, and $\boldsymbol{\theta}_B$ containing the remaining $d-m$ components of $\boldsymbol{\theta}$. We have

$$\boldsymbol{\theta} = (\boldsymbol{\theta}_A, \boldsymbol{\theta}_B)^\mathsf{T} = (\theta_1, \ldots, \theta_m, \theta_{m+1}, \ldots, \theta_d)^\mathsf{T}$$

We want to test the hypothesis $H_0^* : \boldsymbol{\theta}_X \in \Theta_0$ against $H_1^* : \boldsymbol{\theta}_X \notin \Theta_0$, where $\Theta_0 = \{\boldsymbol{\theta} : \boldsymbol{\theta}_A = \boldsymbol{\theta}_{A0}\} \subset \Theta$. We want to know whether the first m components of $\boldsymbol{\theta}_X$ are equal to the vector of constants $\boldsymbol{\theta}_{A0}$ regardless of the other $d-m$ components of $\boldsymbol{\theta}_X$.

This is not a simple null hypothesis because there are many distributions in the model $\mathscr{F}$ that satisfy H_0^*.

All the vectors and matrices appearing in the notation of maximum likelihood estimation theory are decomposed into the first m components (part A) and the remaining $d-m$ components (part B). For example,

$$\widehat{\boldsymbol{\theta}}_n = \begin{pmatrix} \widehat{\boldsymbol{\theta}}_{An} \\ \widehat{\boldsymbol{\theta}}_{Bn} \end{pmatrix}, \qquad \boldsymbol{U}_n(\boldsymbol{\theta}) = \begin{pmatrix} \boldsymbol{U}_{An}(\boldsymbol{\theta}) \\ \boldsymbol{U}_{Bn}(\boldsymbol{\theta}) \end{pmatrix}, \qquad I(\boldsymbol{\theta}) = \begin{pmatrix} I_{AA}(\boldsymbol{\theta}) & I_{AB}(\boldsymbol{\theta}) \\ I_{BA}(\boldsymbol{\theta}) & I_{BB}(\boldsymbol{\theta}) \end{pmatrix}, \quad \text{etc.}$$

The following lemma is useful for inverting the decomposed information matrix.

Lemma A.8 (Block matrix inversion). *Let the matrix*

$$I = \begin{pmatrix} I_{AA} & I_{AB} \\ I_{BA} & I_{BB} \end{pmatrix}$$

be of full rank. Then there exists an inverse matrix to I and it can be expressed as

$$I^{-1} = \begin{pmatrix} I^{AA} & I^{AB} \\ I^{BA} & I^{BB} \end{pmatrix},$$

where

$$\begin{aligned} I^{AA} &= I_{AA.B}^{-1}, \\ I^{AB} &= -I_{AA.B}^{-1} I_{AB} I_{BB}^{-1}, \\ I^{BA} &= -I_{BB.A}^{-1} I_{BA} I_{AA}^{-1}, \\ I^{BB} &= I_{BB.A}^{-1}, \\ I_{AA.B} &= I_{AA} - I_{AB} I_{BB}^{-1} I_{BA} \\ I_{BB.A} &= I_{BB} - I_{BA} I_{AA}^{-1} I_{AB}. \end{aligned}$$ ♢

If the null hypothesis $H_0^* : \boldsymbol{\theta}_X \in \Theta_0$ holds we know that $\boldsymbol{\theta}_{AX} = \boldsymbol{\theta}_{A0}$, but we do not know the value of $\boldsymbol{\theta}_{BX}$. We can estimate $\boldsymbol{\theta}_{BX}$ by the maximum likelihood method applied to the nested submodel

$$\mathscr{F}_0 = \{\text{distributions with density } f(x|(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B)),\ \boldsymbol{\theta}_A = \boldsymbol{\theta}_{A0},\ \boldsymbol{\theta}_B \in \Theta_B \subseteq \mathbb{R}^{d-m}\},$$

with $d-m$ unknown parameters.

Denote the maximum likelihood estimator of $\boldsymbol{\theta}_X$ in the submodel $\mathscr{F}_0$ by $\widetilde{\boldsymbol{\theta}}_n = \begin{pmatrix} \widetilde{\boldsymbol{\theta}}_{An} \\ \widetilde{\boldsymbol{\theta}}_{Bn} \end{pmatrix}$, where $\widetilde{\boldsymbol{\theta}}_{An} = \boldsymbol{\theta}_{A0}$ and $\widetilde{\boldsymbol{\theta}}_{Bn}$ solves the system of likelihood equations

$$\boldsymbol{U}_{Bn}(\boldsymbol{\theta}_{A0}, \widetilde{\boldsymbol{\theta}}_{Bn}) = \mathbf{0}.$$

The Fisher information matrix for $\boldsymbol{\theta}_B$ in this model is $I_{BB}(\boldsymbol{\theta}_X)$.

By Theorems A.3 and A.4 applied to the submodel $\mathscr{F}_0$, we get

$$\frac{1}{\sqrt{n}}\boldsymbol{U}_{Bn}(\boldsymbol{\theta}_X) \xrightarrow{\mathsf{D}} \mathsf{N}_{d-m}(\mathbf{0}, I_{BB}(\boldsymbol{\theta}_X))$$

and

$$\sqrt{n}(\widetilde{\boldsymbol{\theta}}_{Bn} - \boldsymbol{\theta}_{BX}) \xrightarrow{\mathsf{D}} \mathsf{N}_{d-m}(\mathbf{0}, I_{BB}^{-1}(\boldsymbol{\theta}_X)).$$

On the other hand, Theorems A.3 and A.4 and Lemma A.8 applied to the larger model imply

$$\frac{1}{\sqrt{n}}\boldsymbol{U}_{Bn}(\boldsymbol{\theta}_X) \xrightarrow{\mathsf{D}} \mathsf{N}_{d-m}(\mathbf{0}, I_{BB}(\boldsymbol{\theta}_X))$$

and

$$\sqrt{n}(\widehat{\boldsymbol{\theta}}_{Bn} - \boldsymbol{\theta}_{BX}) \xrightarrow{\mathsf{D}} \mathsf{N}_{d-m}(\mathbf{0}, I_{BB.A}^{-1}(\boldsymbol{\theta}_X)),$$

where (dropping the arguments $\boldsymbol{\theta}_X$)

$$I_{BB.A}^{-1} = (I_{BB} - I_{BA}I_{AA}^{-1}I_{AB})^{-1} \geq I_{BB}^{-1}.$$

Thus, the asymptotic variance of the MLE of the parameter $\boldsymbol{\theta}_{BX}$ depends on whether or not $\boldsymbol{\theta}_{AX}$ is known. If $\boldsymbol{\theta}_{AX}$ is known (which is true if H_0^* holds), the asymptotic variance of the MLE $\widetilde{\boldsymbol{\theta}}_{Bn}$ is generally larger than the asymptotic variance of the MLE $\widehat{\boldsymbol{\theta}}_{Bn}$ that does not assume a known $\boldsymbol{\theta}_{AX}$.

However, when $I_{BA} = 0$ (the estimators of $\boldsymbol{\theta}_{AX}$ and $\boldsymbol{\theta}_{BX}$ are asymptotically independent), then the asymptotic variances of $\widetilde{\boldsymbol{\theta}}_{Bn}$ and $\widehat{\boldsymbol{\theta}}_{Bn}$ are the same. Then it does not matter whether or not $\boldsymbol{\theta}_{AX}$ is known.

Let us generalize the three test statistics introduced in Definition A.5 of the previous section to testing the composite hypothesis $H_0^* : \boldsymbol{\theta}_X \in \Theta_0$ against $H_1^* : \boldsymbol{\theta}_X \notin \Theta_0$, where $\Theta_0 = \{\boldsymbol{\theta} : \boldsymbol{\theta}_A = \boldsymbol{\theta}_{A0}\} \subset \Theta$.

Definition A.6.

(i) The statistic

$$\lambda_n^* = \frac{L_n(\widehat{\boldsymbol{\theta}}_n)}{L_n(\widetilde{\boldsymbol{\theta}}_n)}$$

is called *the likelihood ratio*.

(ii) The statistic

$$W_n^* = n(\widehat{\boldsymbol{\theta}}_{An} - \boldsymbol{\theta}_{A0})^\top \widehat{I}_{AA.B}(\widehat{\boldsymbol{\theta}}_n)(\widehat{\boldsymbol{\theta}}_{An} - \boldsymbol{\theta}_{A0})$$

is called *the Wald statistic*.

(iii) The statistic

$$R_n^* = \frac{1}{n}\boldsymbol{U}_n(\widetilde{\boldsymbol{\theta}}_n)^\top \widehat{I}_n^{-1}(\widetilde{\boldsymbol{\theta}}_n)\boldsymbol{U}_n(\widetilde{\boldsymbol{\theta}}_n)$$

is called *the Rao (score) statistic*. ∇

Note.

- Obviously, $\lambda_n^* \geq 1$.
- The expression $\widehat{I}_{AA.B}$ in the Wald statistic means the inverse of the upper left block of the the matrix $\widehat{I}_n^{-1}$.
- Since $\boldsymbol{U}_{Bn}(\widetilde{\boldsymbol{\theta}}_n) = \mathbf{0}$, the Rao statistic can be written as

$$R_n^* = \frac{1}{n}\boldsymbol{U}_{An}(\widetilde{\boldsymbol{\theta}}_n)^\top \widehat{I}_{AA.B}^{-1}(\widetilde{\boldsymbol{\theta}}_n)\boldsymbol{U}_{An}(\widetilde{\boldsymbol{\theta}}_n).$$

- The Rao statistic does not require the calculation of the MLE $\widehat{\boldsymbol{\theta}}_n$ in the larger model, it only needs the MLE $\widetilde{\boldsymbol{\theta}}_n$ in the submodel. This is often much easier to get.

Theorem A.9. *Let the null hypothesis $H_0^* : \boldsymbol{\theta}_X \in \Theta_0$, where $\Theta_0 = \{\boldsymbol{\theta} : \boldsymbol{\theta}_A = \boldsymbol{\theta}_{A0}\}$, hold. Then*

(i)

$$2\log\lambda_n^* = 2(\ell_n(\widehat{\boldsymbol{\theta}}_n) - \ell_n(\widetilde{\boldsymbol{\theta}}_n)) \xrightarrow{D} \chi_m^2;$$

(ii)

$$W_n^* \xrightarrow{D} \chi_m^2;$$

(iii)

$$R_n^* \xrightarrow{D} \chi_m^2.$$ ◇

Note. Under H_0^*, we expect $\widehat{\boldsymbol{\theta}}_n$ to be close to $\widetilde{\boldsymbol{\theta}}_n$, $L_n(\widehat{\boldsymbol{\theta}}_n)$ to be close to $L_n(\widetilde{\boldsymbol{\theta}}_n)$, and $\boldsymbol{U}_n(\widetilde{\boldsymbol{\theta}}_n)$ to be close to $\mathbf{0}$. The large values of the three test statistics testify against the null hypothesis.

Corollary. Let $\chi_m^2(1-\alpha)$ be $(1-\alpha)$-quantile of the χ_m^2 distribution. Consider tests of $H_0^* : \boldsymbol{\theta}_X \in \Theta_0$, where $\Theta_0 = \{\boldsymbol{\theta} : \boldsymbol{\theta}_A = \boldsymbol{\theta}_{A0}\}$, against $H_1^* : \boldsymbol{\theta}_X \notin \Theta_0$ given by the rule: reject H_0^* in favor of H_1^* if

(i) $2\log\lambda_n^* \geq \chi_m^2(1-\alpha)$ *(the likelihood ratio test)*
(ii) $W_n^* \geq \chi_m^2(1-\alpha)$ *(the Wald test)*

(iii) $R_n^* \geq \chi^2_m(1-\alpha)$ *(the score test)*

Then each of these three tests has asymptotically (for $n \to \infty$) the level α.

Note. The number of degrees of freedom in the reference χ^2_m distribution is equal to the number of tested parameters.

Note. These three tests are asymptotically equivalent under the null hypothesis as well as under local alternatives. With small or moderate sample sizes, the likelihood ratio test has the best properties and the Wald test is the worst of the three. In practical applications, the likelihood ratio test should be preferred.

Note. Let $m = 1$, $\boldsymbol{\theta}_{AX} = \theta_{Xj}$, and $\boldsymbol{\theta}_{A0} = 0$. Consider the test of the hypothesis $H_0^* : \theta_{Xj} = 0$ against $H_1^* : \theta_{Xj} \neq 0$ (zero value of the j-th parameter in the presence of other parameters that are unspecified by the hypothesis). Then the Wald statistic can be written as

$$W_n = \left[\frac{\widehat{\theta}_{jn}}{\sqrt{n^{-1}\widehat{I}^{-1}_{jj}}} \right]^2,$$

where $n^{-1}\widehat{I}^{-1}_{jj}$ is the estimator of the asymptotic variance of $\widehat{\theta}_{jn}$. This is the square of the test statistic that statistical software typicaly evaluates to test zero value of a single model parameter.

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