Generalized Linear Models:

An Introduction based on @

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Introduction

- This course will provide an introduction into the concepts of generalized linear models (GLM's).
- This class extends the class of linear models (LM's) to regression models for non-normal data.
- Special interest will be on binary data (logistic regression) and count data (log-linear models).
- All models will be handled by using functions like lm, anova, or glm.

Plan

- Linear Models (LM's): Recap of Results
- Box-Cox Transformation Family: Extending the LM
- Generalized Linear Models (GLM's): An Introduction
- Linear Exponential Family (LEF): Properties and Members
- GLM's: Parameter Estimates
- GLM's: glm(.) Function
- Gamma Regression Models
- Logistic Regression (Binomial Responses)
- Log-linear Model (Poisson Responses)
- Multinomial Response Models
- Quasi-Likelihood Models (Overdispersion)

Goal of regression models is to determine how a **response variable** depends on **covariates**. A special class of regression models are linear models. The general setup is given by

- Data $(Y_i, x_{i1}, \dots, x_{i,p-1}), i = 1, \dots, n$
- Response $\mathbf{y} = (y_1, \dots, y_n)^{\top}$ (random variable)
- Covariates $\mathbf{x}_i = (x_{i1}, \dots, x_{i,p-1})^{\top}$ (fixed, known)

Data Example: Life Expectancies

Source: The World Bank makes available tons of great data from the World Development Indicators that are available within @

```
> install.packages('WDI'); library(WDI)
> WDIsearch('gdp') # gives a list of available data about gdp
> d <- WDI(indicator='NY.GDP.PCAP.KD', country=c('AT', 'US'),</pre>
+ start=1960, end=2012)
> head(d)
 iso2c country NY.GDP.PCAP.KD year
    AT Austria 41246.57 2013
2 AT Austria 41366.52 2012
3 AT Austria 41120.22 2011
4 AT Austria 39972.94 2010
5 AT Austria 39350.17 2009
6
  AT Austria 41043.25 2008
```

Data Example: Life Expectancies

Data on temperature are available at *The World Bank, Climate Change Knowledge Portal: Historical Data*

```
> install.packages('gdata')
# also needs Perl (for MS Windows) to be installed
# also needs java with the same structure as R (32/64 bit)
> library(gdata)
> temp.xls<-"http://databank.worldbank.org/data/download/catalog
             cckp_historical_data_0.xls"
> myperl <- "c:/Strawberry/perl/bin/perl.exe"</pre>
> sheetCount(temp.xls, perl=myperl)
Downloading...
trying URL 'http://databank.worldbank.org/data/.../*.xls'
Content type 'application/vnd.ms-excel' length 378368 bytes
opened URL
downloaded 369 Kb
```

Done.

Data Example: Life Expectancies

```
> temp <- read.xls(temp.xls, sheet="Country_temperatureCRU",</pre>
+
                  perl=myperl)
> temp.data <- temp[ , c("ISO_3DIGIT", "Annual_temp")]</pre>
> colnames(temp.data) <- c("iso3c", "temp")</pre>
> head(temp.data)
 iso3c
           temp
  AFG 12.92
2
 AGO 21.51
3
  ALB 11.27
4
   ARE 26.83
5 ARG
         14.22
6
   ARM
            6.37
```

Data Example: Life Expectancies Data we are interested in (from 2010):

- life.exp at birth, total (years)
- urban population (percent)
- physicians (per 1,000 people)
- temp annual mean (Celsius)

Which is the response and which are covariates?

Gaussian Linear Model:

$$y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_{p-1} x_{i,p-1} + \epsilon_i$$
, $\epsilon_i \stackrel{iid}{\sim} \text{Normal}(0, \sigma^2)$,

with unknown regression parameters $\beta_0, \beta_1, \dots, \beta_{p-1}$ (intercept β_0 , slopes β_j , $j=1,\dots,p-1$) and unknown (homogenous) **error** variance σ^2 .

This is equivalent with $y_i \stackrel{ind}{\sim} \text{Normal}(E(y_i), \text{var}(y_i))$, where

$$E(y_i) = \mu_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_{p-1} x_{i,p-1}$$

is a linear function in the parameters and

$$var(y_i) = \sigma^2$$
, $i = 1, ..., n$

describes a homoscedastic scenario.



Matrix Notation: we define

$$\mathbf{y} = (y_1, \dots, y_n)^\top, \quad \boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_n)^\top, \\ \boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_{p-1})^\top, \quad \mathbf{x}_i = (1, x_{i1}, \dots, x_{i,p-1})^\top, \\ \mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top$$

and write the Gaussian regression models as

$$y = X\beta + \epsilon$$

with

$$\mathsf{E}(\mathsf{y}) = \boldsymbol{\mu} = \mathsf{X}\boldsymbol{\beta}$$

and

$$var(\mathbf{y}) = \sigma^2 \mathbf{I}_n$$
.

Here I_n denotes the $(n \times n)$ identity matrix and the $(n \times p)$ matrix **X** is also called **Design Matrix**.

Exploratory Data Analysis (EDA):

- Check out the **ranges** of the response and covariates. For **discrete** covariates (with sparse factor levels) we consider **grouping** the levels.
- Plot covariates against response. Scatter plot should reflect **linear** relationships otherwise we consider **transformations**.
- To check if the constant variance assumption is reasonable, the points of the scatter plot of covariates against the responses should be contained in a **horizontal band**.

Data Example: Life Expectancies (EDA)

> summary(mydata[, c(5, 6, 8, 10)])

```
      life.exp
      urban
      physicians
      temp

      Min.
      :44.84
      Min.
      :0.09092
      Min.
      :0.008
      Min.
      :-7.14

      1st Qu.:62.16
      1st Qu.:0.37396
      1st Qu.:0.272
      1st Qu.:10.15

      Median
      :71.83
      Median
      :0.56297
      Median
      :1.764
      Median
      :21.58

      Mean
      :69.11
      Mean
      :0.55892
      Mean
      :1.871
      Mean
      :18.06

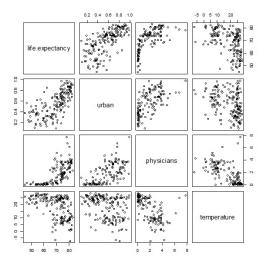
      3rd Qu.:76.10
      3rd Qu.:0.74453
      3rd Qu.:3.000
      3rd Qu.:25.05

      Max.
      :82.84
      Max.
      :0.98655
      Max.
      :7.739
      Max.
      :28.30

      NA's
      :1
      NA's
      :39
```

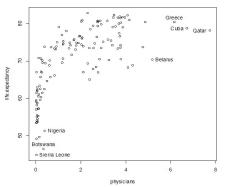
Data Example: Life Expectancies (EDA)

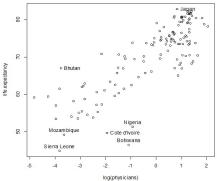
> plot(mydata[, c(5, 6, 8, 10)])



Data Example: Life Expectancies (Transformations)

```
plot(physicians, life.exp)
plot(log(physicians), life.exp)
```





Parameter Estimation: β

Idea of Least Squares: minimize the sum of squared errors, i.e.

$$SSE(\boldsymbol{\beta}) = \sum_{i=1}^{n} (y_i - \mathbf{x}_i^{\top} \boldsymbol{\beta})^2$$

Equivalent with **Maximum Likelihood**: maximize the sample log-likelihood function

$$\ell(\boldsymbol{\beta}|\mathbf{y}) = \sum_{i=1}^{n} \left(\log \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} (y_i - \mathbf{x}_i^{\top} \boldsymbol{\beta})^2 \right)$$

LSE/MLE **Solution**: $\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y}$

For $y_i \stackrel{ind}{\sim} \text{Normal}(\mathbf{x}_i^{\top} \boldsymbol{\beta}, \sigma^2)$ we have

$$\hat{\boldsymbol{\beta}} \sim \text{Normal}(\boldsymbol{\beta}, \sigma^2(\mathbf{X}^{\top}\mathbf{X})^{-1})$$

Parameter Estimation: σ^2

Maximum Likelihood Estimator:

$$\hat{\sigma}^2 = \frac{1}{n} SSE(\hat{\boldsymbol{\beta}}) = \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{x}_i^{\top} \hat{\boldsymbol{\beta}})^2, \qquad E(\hat{\sigma}^2) = \left(1 - \frac{p}{n}\right) \sigma^2$$

is biased. An **unbiased** variance estimator is (df corrected)

$$S^2 = \frac{1}{n-p} \operatorname{SSE}(\hat{\boldsymbol{\beta}})$$

For $y_i \stackrel{ind}{\sim} \text{Normal}(\mathbf{x}_i^{\top} \boldsymbol{\beta}, \sigma^2)$ we get

$$SSE(\hat{\boldsymbol{\beta}})/\sigma^2 \sim \chi^2_{n-p}$$

and $SSE(\hat{\beta})$ is **independent** of $\hat{\beta}$.



ANalysis Of VAriance (ANOVA): let $\hat{\mu}_i = \mathbf{x}_i^{\top} \boldsymbol{\beta}$, then

$$\sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum_{i=1}^{n} (\hat{\mu}_i - \bar{y})^2 + \sum_{i=1}^{n} (y_i - \hat{\mu}_i)^2$$
SST SSR(\hat{\hat{\hat{\beta}}}) SSE(\hat{\hat{\hat{\hat{\beta}}}})

Total SS equals (maxim.) Regression SS plus (minim.) Error SS

Thus, the proportion of variability explained by the regression model is described by the **coefficient of determination**

$$R^2 = \frac{\mathsf{SSR}(\hat{\boldsymbol{\beta}})}{\mathsf{SST}} = 1 - \frac{\mathsf{SSE}(\hat{\boldsymbol{\beta}})}{\mathsf{SST}} \in (0, 1)$$

To penalize for model complexity p we use its **adjusted** version

$$R_{adj}^2 = 1 - \frac{SSE(\hat{\beta})/(n-p)}{SST/(n-1)} \not\in (0,1)$$

Hypothesis Tests: t-Test

If the model is correctly stated then

$$\hat{\boldsymbol{\beta}} \sim \text{Normal}(\boldsymbol{\beta}, \sigma^2(\mathbf{X}^{\top}\mathbf{X})^{-1})$$

Thus, for each **slope** parameter β_j , j = 1, ..., p - 1, we have

$$\hat{eta}_j \sim \mathsf{Normal}(eta_j, \sigma^2(\mathbf{X}^{ op}\mathbf{X})_{j+1, j+1}^{-1})$$

and therefore

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{\sigma^2(\mathbf{X}^\top \mathbf{X})_{j+1,j+1}^{-1}}} \sim \mathsf{Normal}(0,1)$$

Since S^2 and $\hat{\beta}$ are independent, replacing σ^2 by S^2 results in

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{S^2(\mathbf{X}^\top \mathbf{X})_{j+1,j+1}^{-1}}} \sim t_{n-p}$$

Hypothesis Tests: t-Test

$$\frac{\hat{\beta}_j - \beta_j}{\sqrt{S^2(\mathbf{X}^{\top}\mathbf{X})_{j+1,j+1}^{-1}}} \sim t_{n-p}$$

Therefore, we can test the relevance of a **single predictor** x_j by

$$H_0: \beta_j = 0$$
 vs $H_1: \beta_j \neq 0$

and use the well-known test statistic

$$\frac{\mathsf{Estimate}}{\mathsf{Std. Error}} = \frac{\hat{\beta}_j}{\sqrt{S^2(\mathbf{X}^\top \mathbf{X})_{j+1,j+1}^{-1}}} \stackrel{H_0}{\sim} t_{n-p}$$

Hypothesis Tests: F-Test

If a predictor is a **factor** with k levels (e.g., continent: Europe, Africa, America, Asia), then we usually define a baseline category (e.g. Europe) and consider the model

$$\mu = \beta_0 + \beta_{Af}I(Africa) + \beta_{Am}I(America) + \beta_{As}I(Asia)$$

To check if the predictor continent is irrelevant we have to test k-1 parameters

$$H_0: \beta_{Af} = \beta_{Am} = \beta_{As} = 0$$
 vs $H_1: not H_0$

Fitting the model twice, under H_0 and under H_1 , results in $SSR(\hat{\beta}_0)$ and $SSR(\hat{\beta}_1)$ and we get the **test statistic**

$$\frac{\left(\operatorname{SSR}(\hat{\boldsymbol{\beta}}_1) - \operatorname{SSR}(\hat{\boldsymbol{\beta}}_0)\right)/(k-1)}{\operatorname{SSE}(\hat{\boldsymbol{\beta}}_1)/(n-p)} \stackrel{H_0}{\sim} F_{k-1,n-p}.$$



Weighted Least Squares in case of heteroscedastic errors, i.e.

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \text{Normal}(\mathbf{0}, \sigma^2 \mathbf{W}), \quad \mathbf{W} = \text{diag}(w_1, \dots, w_n)$$

The MLE (weighted LSE) of β is given by

$$\hat{oldsymbol{eta}} = (\mathbf{X}^{ op}\mathbf{W}^{-1}\mathbf{X})^{-1}\mathbf{X}^{ op}\mathbf{W}^{-1}\mathbf{y}$$

with

$$\mathsf{E}(\hat{\boldsymbol{\beta}}) = \boldsymbol{\beta}$$
 and $\mathsf{var}(\hat{\boldsymbol{\beta}}) = \sigma^2 (\mathbf{X}^{\top} \mathbf{W}^{-1} \mathbf{X})^{-1}$

The MLE of σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n \frac{(y_i - \hat{\mu}_i)^2}{w_i} = \frac{1}{n} \mathbf{r}^\top \mathbf{W}^{-1} \mathbf{r}$$

with the vector of raw residuals ${f r}={f y}$ $+\hat{m \mu}$.

Data Example: Life Expectancies

```
> mod <- lm(life.exp ~ urban + physicians + temp)</pre>
> summary(mod)
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 61.49091 2.21534 27.757 < 2e-16 ***
urban 15.06895 2.94544 5.116 1.1e-06 ***
physicians 1.87133 0.46933 3.987 0.000111 ***
temp -0.19079 0.07287 -2.618 0.009896 **
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 5.874 on 129 degrees of freedom
  (39 observations deleted due to missingness)
Multiple R-squared: 0.5872, Adjusted R-squared: 0.5776
F-statistic: 61.17 on 3 and 129 DF, p-value: < 2.2e-16
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```

Data Example: Life Expectancies

Coefficients:

Estimate Std. Error t value Pr(>|t|)

All predictors are significant (on a 5% level). Only temp has a negative effect.

Data Example: Life Expectancies

Residual standard error: 5.874 on 129 degrees of freedom (39 observations deleted due to missingness)

Multiple R-squared: 0.5872, Adjusted R-squared: 0.5776

F-statistic: 61.17 on 3 and 129 DF, p-value: < 2.2e-16

Under the model, the estimated standard error of the response is 5.874 (years). We have n-p=129 and p-1=3 predictors.

Almost 60% of the total variability is explained by this model. The adjusted version of R^2 is 0.5776.

We finally test that **all three** predictors are irrelevant. The associated F-test clearly rejects this hypothesis.

Data Example: Life Expectancies (log(physicians))

Predictor temp is no longer significant!

Data Example: Life Expectancies (log(physicians))

```
Residual standard error: 4.958 on 129 degrees of freedom (39 observations deleted due to missingness)

Multiple R-squared: 0.7059, Adjusted R-squared: 0.6991

F-statistic: 103.2 on 3 and 129 DF, p-value: < 2.2e-16
```

Standard error is much smaller now as before (± 5 years)!

Even 70% of the total variability is now explained by this model.

Same conclusion based on global F-test as in previous model.

> anova(mod.log)

Data Example: Life Expectancies (ANOVA)

Data Example: Life Expectancies (ANOVA)

Remember the SST decomposition under the **Model** $\mu = X\beta$:

$$SST = SSR(\hat{\beta}) + SSE(\hat{\beta})$$

Information about this is contained in the **ANOVA Table**:

Source		Sum of Squares/SS		F
Regression	<i>p</i> – 1	$SSR(\hat{\beta}) =$	$MSR(\hat{\boldsymbol{eta}}) =$	
		SST – SSE($\hat{\beta}$)	$SSR(\hat{\boldsymbol{eta}})/(p-1)$	$\frac{MSR(\hat{\boldsymbol{\beta}})}{MSE(\hat{\boldsymbol{\beta}})}$
Error	n-p	SSE(Â)	$MSE(\hat{\boldsymbol{\beta}}) = SSE(\hat{\boldsymbol{\beta}})/(n-p)$	
Total	<i>n</i> – 1	SST		

Data Example: Life Expectancies (ANOVA)

Null Model: assuming an **iid** random sample $(E(y_i) = \beta_0 \cdot 1)$, results in $SSE(\hat{\beta}_0) = \sum_i (y_i - \hat{\beta}_0)^2$ where $\hat{\beta}_0 = \bar{y}$. Thus, $SSE(\hat{\beta}_0) = \sum_i (y_i - \bar{y})^2 \equiv SST$ in this case.

Nested Model: we assume that

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\epsilon}$$
, and test on $H_0: \boldsymbol{\beta}_2 = \mathbf{0}$

with $\dim(\boldsymbol{\beta}_1) = p_1$ (including the intercept) and $\dim(\boldsymbol{\beta}_2) = p_2$ (additional slopes). The corresponding SSR and SSE terms are

$$SSR(\hat{\boldsymbol{\beta}}_1) = \sum_{i=1}^n (\mathbf{x}_i^{\top} \hat{\boldsymbol{\beta}}_1 - \bar{y})^2, \qquad SSE(\hat{\boldsymbol{\beta}}_1) = \sum_{i=1}^n (y_i - \mathbf{x}_i^{\top} \hat{\boldsymbol{\beta}}_1)^2$$

Data Example: Life Expectancies (ANOVA)

Sequentially adding the term \mathbf{X}_2 in the model where \mathbf{X}_1 is already included results in

Source	df	Sum of Squares/SS	MSS	F
X ₁	$p_1 - 1$	$SSR(\hat{oldsymbol{eta}}_1)$	$ MSR(\hat{\boldsymbol{\beta}}_1) = \\ \frac{SSR(\hat{\boldsymbol{\beta}}_1)}{p_1 - 1} $	$\frac{MSR(\hat{\boldsymbol{\beta}}_1)}{MSE(\hat{\boldsymbol{\beta}})}$
$\mathbf{X}_2 \mathbf{X}_1$	<i>p</i> ₂	$SSR(\hat{\boldsymbol{\beta}}_2 \hat{\boldsymbol{\beta}}_1) = SSR(\hat{\boldsymbol{\beta}}) - SSR(\hat{\boldsymbol{\beta}}_1)$	$\frac{MSR(\hat{\boldsymbol{\beta}}_2 \hat{\boldsymbol{\beta}}_1) = }{\frac{SSR(\hat{\boldsymbol{\beta}}_2 \hat{\boldsymbol{\beta}}_1)}{p_2}}$	$\frac{MSR(\hat{\boldsymbol{\beta}}_2 \hat{\boldsymbol{\beta}}_1)}{MSE(\hat{\boldsymbol{\beta}})}$
Error	n – p	SSE($\hat{\boldsymbol{\beta}}$)	$MSE(\hat{\boldsymbol{\beta}}) = SSE(\hat{\boldsymbol{\beta}})/(n-p)$	
Total	<i>n</i> – 1	SST		

Data Example: Life Expectancies (ANOVA)

We now assume that the model $\mathbf{y} = \beta_0 + \mathbf{X}_1 \boldsymbol{\beta}_1 + \mathbf{X}_2 \boldsymbol{\beta}_2 + \boldsymbol{\epsilon}$ holds.

Test 1: test statistic

$$F = \frac{\mathsf{MSR}(\hat{\boldsymbol{\beta}}_1 | \hat{\boldsymbol{\beta}}_0)}{\mathsf{MSE}(\hat{\boldsymbol{\beta}})}$$

tests the model improvement when adding the predictors in \mathbf{X}_1 to the iid model with only β_0 .

Test 2: test statistic

$$F = \frac{\mathsf{MSR}(\hat{\boldsymbol{\beta}}_2|\hat{\boldsymbol{\beta}}_1, \hat{\beta}_0)}{\mathsf{MSE}(\hat{\boldsymbol{\beta}})}$$

tests the model improvement when adding the predictors in \mathbf{X}_2 to the model with \mathbf{X}_1 and $\boldsymbol{\beta}_0$ already contained.

> anova(mod.log)

Analysis of Variance Table

Data Example: Life Expectancies (ANOVA)

Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1

Each further predictor that enters the model significantly improves the model fit.

Linear Models: Restrictions

Problems:

- $y_i \not\sim \text{Normal}(\mathsf{E}(y_i), \text{var}(y_i))$
- $\mathsf{E}(y_i) \neq \mathbf{x}_i^{\mathsf{T}} \boldsymbol{\beta} \in \mathbb{R}$
- $var(y_i) \neq \sigma^2$ equal (homoscedastic) $\forall i = 1, ..., n$

Remedies:

- transform y_i such that $g(y_i) \stackrel{ind}{\sim} \text{Normal}(\mathbf{x}_i^{\top} \boldsymbol{\beta}, \sigma^2)$
- utilize a GLM where $y_i \stackrel{ind}{\sim} \mathsf{LEF}(g^{-1}(\mathbf{x}_i^{\top} \boldsymbol{\beta}), \phi V(\mu_i))$

Box-Cox Transformation

Define for **positive** Responses (y > 0)

$$y(\lambda) = \begin{cases} \frac{y^{\lambda} - 1}{\lambda}, & \text{if } \lambda \neq 0, \\ \log y, & \text{if } \lambda = 0, \end{cases}$$

 $y(\lambda) \to \log y$ for $\lambda \to 0$, such that $y(\lambda)$ is continuous in λ .

Assumption: there is a value λ for which

$$y_i(\lambda) \stackrel{ind}{\sim} \text{Normal}\Big(\mu_i(\lambda) = \mathbf{x}_i^{\top} \boldsymbol{\beta}(\lambda), \sigma^2(\lambda)\Big)$$

Compute MLEs with respect to the sample density of the untransformed response *y*.

Box-Cox Transformation

Density Transformation Theorem: If $g(Y) \sim F_{g(Y)}(y)$ holds for a continuous r.v. and $g(\cdot)$ is a monotone function, then the untransformed r.v. Y has cdf

$$F_Y(y) = \Pr(Y \le y) = \Pr(g(Y) \le g(y)) = F_{g(Y)}(g(y)).$$

Thus, the density of Y is

$$f_Y(y) = \frac{\partial F_{g(Y)}(g(y))}{\partial y} = f_{g(Y)}(g(y)) \cdot \left| \frac{\partial g(y)}{\partial y} \right|$$

with Jacobian $\left| \frac{\partial g(y)}{\partial y} \right|$.

Box-Cox Transformation

Density of untransformed y is

$$f(y|\lambda,\mu(\lambda),\sigma^{2}(\lambda)) = \begin{cases} \frac{1}{\sqrt{2\pi\sigma^{2}(\lambda)}} \exp\left(-\frac{\left(\frac{(y^{\lambda}-1)}{\lambda}-\mu(\lambda)\right)^{2}}{2\sigma^{2}(\lambda)}\right) y^{\lambda-1}, & \lambda \neq 0, \\ \frac{1}{\sqrt{2\pi\sigma^{2}(\lambda)}} \exp\left(-\frac{(\log y - \mu(\lambda))^{2}}{2\sigma^{2}(\lambda)}\right) y^{-1}, & \lambda = 0. \end{cases}$$

• If $\lambda \neq 0$ and $\mu(\lambda) = \mathbf{x}^{\top} \boldsymbol{\beta}(\lambda)$ then

$$f(y|\lambda, \mu(\lambda), \sigma^{2}(\lambda)) = \frac{1}{\sqrt{2\pi\lambda^{2}\sigma^{2}(\lambda)}} \exp\left(-\frac{\left(y^{\lambda} - 1 - \lambda \mathbf{x}^{\top}\boldsymbol{\beta}(\lambda)\right)^{2}}{2\lambda^{2}\sigma^{2}(\lambda)}\right) |\lambda| y^{\lambda-1}.$$

Box-Cox Transformation

Using $\beta_0 = 1 + \lambda \beta_0(\lambda)$, $\beta_j = \lambda \beta_j(\lambda)$, j = 1, ..., p - 1, and $\sigma^2 = \lambda^2 \sigma^2(\lambda)$ then

$$f(y|\lambda, \mu(\lambda), \sigma^{2}(\lambda)) = \frac{1}{\sqrt{2\pi\lambda^{2}\sigma^{2}(\lambda)}} \exp\left(-\frac{(y^{\lambda} - 1 - \lambda \mathbf{x}^{\top}\boldsymbol{\beta}(\lambda))^{2}}{2\lambda^{2}\sigma^{2}(\lambda)}\right) |\lambda| y^{\lambda-1}$$
$$f(y|\lambda, \boldsymbol{\beta}, \sigma^{2}) = \frac{1}{\sqrt{2\pi\sigma^{2}}} \exp\left(-\frac{(y^{\lambda} - \mathbf{x}^{\top}\boldsymbol{\beta})^{2}}{2\sigma^{2}}\right) |\lambda| y^{\lambda-1}.$$

• If $\lambda = 0$, let $\beta_j = \beta_j(\lambda)$, j = 0, ..., p - 1, and $\sigma^2 = \sigma^2(\lambda)$

$$f(y|0, \boldsymbol{\beta}, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(\log y - \mathbf{x}^{\top}\boldsymbol{\beta})^2}{2\sigma^2}\right) y^{-1}.$$

If λ would be known, then the MLE could be easily computed!

Box-Cox Transformation

Relevant part of the sample log-likelihood function is

• $\lambda \neq 0$:

$$\ell(\lambda, \boldsymbol{\beta}, \sigma^2 | \mathbf{y}) = -\frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i^{\lambda} - \mathbf{x}_i^{\top} \boldsymbol{\beta})^2 + n \log |\lambda| + (\lambda - 1) \sum_{i=1}^n \log y_i$$

• $\lambda = 0$:

$$\ell(0, \boldsymbol{\beta}, \sigma^2 | \mathbf{y}) = -\frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n \left(\log y_i - \mathbf{x}_i^{\mathsf{T}} \boldsymbol{\beta} \right)^2 - \sum_{i=1}^n \log y_i$$



Box-Cox Transformation: MLE's

If λ would be known, then the MLEs would be

$$\hat{\boldsymbol{\beta}}_{\lambda} = \begin{cases} (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}^{\lambda}, & \lambda \neq 0, \\ (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \log \mathbf{y}, & \lambda = 0, \end{cases}$$

$$\hat{\sigma}_{\lambda}^{2} = \frac{1}{n} SSE_{\lambda}(\hat{\boldsymbol{\beta}}_{\lambda}) = \begin{cases} \frac{1}{n} \sum_{i=1}^{n} (y_{i}^{\lambda} - \mathbf{x}_{i}^{\top} \hat{\boldsymbol{\beta}}_{\lambda})^{2}, & \lambda \neq 0, \\ \frac{1}{n} \sum_{i=1}^{n} (\log y_{i} - \mathbf{x}_{i}^{\top} \hat{\boldsymbol{\beta}}_{\lambda})^{2}, & \lambda = 0. \end{cases}$$

Box-Cox Transformation: Profile-Likelihood Estimator

Profile (log-) likelihood function $p\ell(\lambda|\mathbf{y}) = \ell(\lambda, \hat{\boldsymbol{\beta}}_{\lambda}, \hat{\sigma}_{\lambda}^2|\mathbf{y}) =$

$$= \begin{cases} -\frac{n}{2}\log SSE_{\lambda}(\hat{\boldsymbol{\beta}}_{\lambda}) + n\log|\lambda| + (\lambda - 1)\sum_{i=1}^{n}\log y_{i}, & \lambda \neq 0, \\ -\frac{n}{2}\log SSE_{0}(\hat{\boldsymbol{\beta}}_{0}) - \sum_{i=1}^{n}\log y_{i}, & \lambda = 0. \end{cases}$$

This is the sample log-likelihood function that has been already maximized with respect to β and σ^2 .

It only depends on the transformation parameter λ .

Find the maximum in λ by simply using a grid search strategy.



Box-Cox Transformation: Profile-Likelihood

Likelihood Ratio Test (LRT): $H_0: \lambda = \lambda_0$ versus $H_1: \lambda \neq \lambda_0$. For the LRT statistic it holds that

$$-2\left(\rho\ell(\lambda_0|\mathbf{y})-\rho\ell(\hat{\lambda}|\mathbf{y})\right)\overset{\mathcal{D}}{\rightarrow}\chi_1^2.$$

If $-2(p\ell(\lambda_0|\mathbf{y}) - p\ell(\hat{\lambda}|\mathbf{y})) \sim \chi_1^2$, a $(1-\alpha)$ confidence interval contains all values λ_0 , for which

$$-\big(\rho\ell(\lambda_0|\mathbf{y})-\rho\ell(\hat{\lambda}|\mathbf{y})\big)<\frac{1}{2}\chi_{1;1-\alpha}^2$$

(notice that $\chi^2_{1;0.95} = 3.841$, $\chi^2_{1;0.99} = 6.635$).

Box-Cox Transformation: Properties

Log-Transformation ($\lambda = 0$): if log $y_i \sim \text{Normal}(\mathbf{x}_i^{\mathsf{T}}\boldsymbol{\beta}, \sigma^2)$ then

median(log
$$y_i$$
) = $\mathbf{x}_i^{\top} \boldsymbol{\beta}$,

$$E(\log y_i) = \mathbf{x}_i^{\top} \boldsymbol{\beta}$$
,

$$var(\log y_i) = \sigma^2$$
.

Untransformed response y_i follows a log-normal distribution with

median
$$(y_i) = \exp(\mathbf{x}_i^{\top} \boldsymbol{\beta}),$$

$$E(y_i) = \exp(\mathbf{x}_i^{\top} \boldsymbol{\beta} + \sigma^2/2) = \exp(\mathbf{x}_i^{\top} \boldsymbol{\beta}) \exp(\sigma^2/2),$$

$$var(y_i) = (\exp(\sigma^2) - 1) \exp(2\mathbf{x}_i^{\top} \boldsymbol{\beta} + \sigma^2).$$

- **Additive** model for mean and median of $\log y_i$ corresponds to a **multiplicative** model for mean and median of y_i .
- $E(y_i)$ is $1 < \exp(\sigma^2/2)$ times its median (y_i) .
- $\operatorname{var}(y_i)$ is no longer constant for $i=1,\dots,n$,

Box-Cox Transformation: Properties

Untransformed response y_i follows a distribution with

median
$$(y_i) = \mu_i^{1/\lambda}$$
,
$$E(y_i) \approx \mu_i^{1/\lambda} \left(1 + \sigma^2 (1 - \lambda) / (2\lambda^2 \mu_i^2) \right),$$

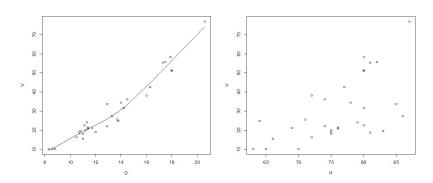
$$var(y_i) \approx \mu_i^{2/\lambda} \sigma^2 / (\lambda^2 \mu_i^2).$$

Girth (diameter), Height and Volume for n=31 Black Cherry Trees available in \mathbf{Q} .

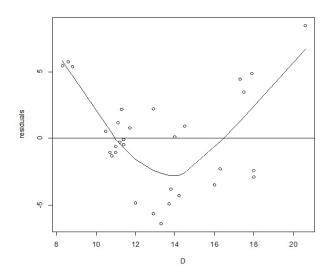
Relationship between volume V in feet³, height H in feet and diameter D in inches (1 inch = 2.54 cm, 12 inches = 1 foot).

```
> H <- trees$Height; D <- trees$Girth; V <- trees$Volume
```

- > plot(D, V); lines(lowess(D, V)) # curvature (wrong scale?)
- > plot(H, V) # increasing variance?

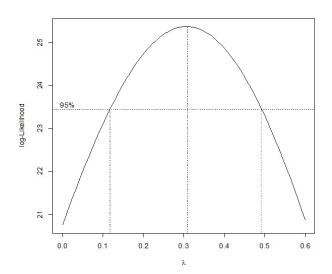


- > plot(D, residuals(mod), ylab="residuals"); abline(0, 0)
- > lines(lowess(D, residuals(mod))) # sink in the middle



```
> library(MASS)
> bc<-boxcox(V~H+D,lambda=seq(0.0,0.6,length=100),plotit=FALSE)
> ml.index <- which(bc$y == max(bc$y))
> bc$x[ml.index]
[1] 0.3090909
```

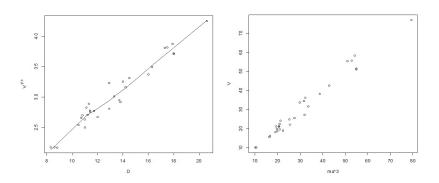
 $> boxcox(V^{H+D}, lambda = seq(0.0, 0.6, len = 18)) # plot it now$



Is volume cubic in height and diameter?

```
> plot(D, V^(1/3), ylab=expression(V^{1/3}))
> lines(lowess(D, V^(1/3))) # curvature almost gone
> (mod1 <- lm(V^(1/3) ~ H + D))
Coefficients:
(Intercept)
   -0.08539 0.01447 0.15152
For fixed \lambda = 1/3 we have median (V) = \hat{\mu}_{1/3}^3 where
\mathsf{E}(V^{1/3}) = \mu_{1/3}. \hat{\mathsf{E}}(V) = \hat{\mu}_{1/3}^3 (1 + 3\hat{\sigma}_{1/3}^2/\hat{\mu}_{1/3}^2). Compare
responses with estimated medians
```

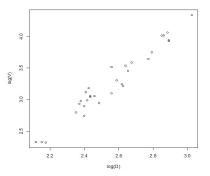
- > mu <- fitted(mod1)
- > plot(mu^3, V) # fitted median modell

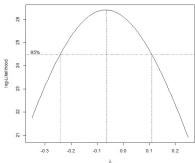


Alternative strategy:

 $> boxcox(V^{\circ}log(H)+log(D), lambda=seq(-0.35,0.25,length=100))$

Remove curvature by a log-transform of all predictors (i.e.,





Which of the models is *better*? Comparison by LRT. Both models are members of the **model family**

$$V^* \sim \text{Normal}(\beta_0 + \beta_1 H^* + \beta_2 D^*, \sigma^2)$$

$$V^* = (V^{\lambda_V} - 1)/\lambda_V$$

$$H^* = (H^{\lambda_H} - 1)/\lambda_H$$

$$D^* = (D^{\lambda_D} - 1)/\lambda_D$$

Compare Profile-Likelihood function in $\lambda_V = 1/3$, $\lambda_H = \lambda_D = 1$ (E($V^{1/3}$) = $\beta_0 + \beta_1 H + \beta_2 D$), with that in $\lambda_V = \lambda_H = \lambda_D = 0$ (E($\log(V)$) = $\beta_0 + \beta_1 \log(H) + \beta_2 \log(D)$).

```
> bc1 <- boxcox(V ~ H + D, lambda = 1/3, plotit=FALSE)
> bc1$y
[1] 25.33313
> bc2 <- boxcox(V ~ log(H) + log(D), lambda = 0, plotit=FALSE)
> bc2$y
[1] 26.11592
```

LRT Statistic: -2(25.333 - 26.116) = 1.566 (not significant).

Remark: Coefficient of $\log(H)$ close to 1 ($\hat{\beta}_1 = 1.117$) and coefficient of $\log(D)$ close to 2 ($\hat{\beta}_2 = 1.983$).

Tree can be represented by a **cylinder** or a **cone**. Volume is $\pi hd^2/4$ (cylinder) or $\pi hd^2/12$ (cone), i.e.

$$\mathsf{E}(\log(V)) = c + 1\log(H) + 2\log(D)$$

with $c = \log(\pi/4)$ (cylinder) or $c = \log(\pi/12)$ (cone).

Attention: D has to be converted from inches to feet $\Rightarrow D/12$ as predictor.

Conversion only influences intercept!

Fix slopes (β_1, β_2) to (1, 2) and estimate only intercept β_0 , i.e. consider the model

$$E(\log(V)) = \beta_0 + 1\log(H) + 2\log(D/12)$$
.

Term $1 \log H + 2 \log(D/12)$ is called **offset** (predictor with fixed parameter 1).

Volume can be better described by a cone than by a cylinder. However, its volume is slightly larger than the one of a cone.

Introduction to GLM's

- In **generalized linear models** (GLM's) we again have independent response variables with covariates.
- While a linear model combines additivity of the covariate effects with the normality of the errors, including variance homogeneity, GLM's don't need to satisfy these requirements. GLM's allow also to handle nonnormal responses such as binomial, Poisson and Gamma.
- Regression parameters are estimated using maximum likelihood.
- Standard reference on GLM's is McCullagh & Nelder (1989).

Introduction to GLM's: Components of a GLM

Response y_i and covariables $\mathbf{x}_i = (1, x_{i1}, \dots, x_{i,p-1})^{\top}$.

1 Random Component: y_i, i = 1,..., n, independent with density from the linear exponential family (LEF), i.e.

$$f(y|\theta,\phi) = \exp\left\{\frac{y\theta - b(\theta)}{\phi} + c(y,\phi)\right\}$$

 $\phi > 0$ is a dispersion parameter and $b(\cdot)$ and $c(\cdot, \cdot)$ are known functions.

- ② Systematic Component: $\eta_i = \eta_i(\boldsymbol{\beta}) = \mathbf{x}_i^{\top} \boldsymbol{\beta}$ is called **linear predictor**, $\boldsymbol{\beta} = (\beta_0, \dots, \beta_{p-1})^{\top}$ are unknown regression parameters
- 3 Parametric Link Component: The **link function** $g(\mu_i) = \eta_i$ combines the linear predictor with the mean of y_i . **Canonical** link function if $\theta = \eta$.

Introduction to GLM's: LM as GLM

 $y_i \sim \text{Normal}(\mathbf{x}_i^{\mathsf{T}}\boldsymbol{\beta}, \sigma^2)$, independent, i = 1, ..., n. Density has LEF form, since

$$f(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2\sigma^2}(y-\mu)^2\right\}$$
$$= \exp\left\{\frac{y\mu - \frac{\mu^2}{2}}{\sigma^2} - \frac{1}{2}\left[\log(2\pi\sigma^2) + \frac{y^2}{\sigma^2}\right]\right\}$$

Defining $\theta = \mu$ and $\phi = \sigma^2$ results in

$$b(\theta) = \frac{\mu^2}{2}$$
 and $c(y, \phi) = -\frac{1}{2} \left[\log(2\pi\sigma^2) + \frac{y^2}{\sigma^2} \right]$

Since $\theta = \mu$, the canonical link $g(\mu) = \mu$ is used in a LM.

Introduction to GLM's: Moments

It can be shown that for the LEF

$$E(y) = b'(\theta) = \mu$$
$$var(y) = \phi b''(\theta) = \phi V(\mu),$$

where $V(\mu) = b''(\theta)$ is called the **variance function**. Thus, we generally consider the model

$$g(\mu) = g(b'(\theta)).$$

Thus, the canonical link is defined as

$$g = (b')^{-1}$$

$$\Rightarrow g(\mu) = \theta = \mathbf{x}^{\top} \boldsymbol{\beta}.$$

A single algorithm can be used to estimate the parameters of an LEM glm using **maximum likelihood**.

The log-likelihood of the sample y_1, \ldots, y_n is

$$\ell(\boldsymbol{\mu}|\mathbf{y}) = \sum_{i=1}^{n} \left\{ \frac{y_i \theta_i - b(\theta_i)}{\phi} + c(y_i, \phi) \right\}$$

The maximum likelihood estimator $\hat{\mu}$ is obtained by solving the score function (chain rule)

$$s(\boldsymbol{\mu}) = \frac{\partial}{\partial \boldsymbol{\mu}} \ell(\boldsymbol{\mu} | \mathbf{y}) = \frac{\partial}{\partial \boldsymbol{\theta}} \ell(\boldsymbol{\mu} | \mathbf{y}) \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{\mu}} = \left(\frac{y_1 - \mu_1}{\phi V(\mu_1)}, \dots, \frac{y_n - \mu_n}{\phi V(\mu_n)} \right)$$

that only depends on a **mean/variance relationship**.

Because of $\mu = \mu(\boldsymbol{\beta})$ the score function for the parameter $\boldsymbol{\beta}$ is (chain rule again)

$$s(\boldsymbol{\beta}) = \frac{\partial}{\partial \boldsymbol{\beta}} \ell(\boldsymbol{\beta}|\mathbf{y}) = \frac{\partial}{\partial \boldsymbol{\theta}} \ell(\boldsymbol{\mu}|\mathbf{y}) \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{\mu}} \frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}} \frac{\partial \boldsymbol{\eta}}{\partial \boldsymbol{\beta}} = \sum_{i=1}^{n} \frac{y_{i} - \mu_{i}}{\phi V(\mu_{i})} \frac{1}{g'(\mu_{i})} \mathbf{x}_{i}$$

which depends again only on the mean/variance relationship.

For the sample y_1, \ldots, y_n we assumed that there is only one **global dispersion parameter** ϕ , i.e. $E(y_i) = \mu_i$, $var(y_i) = \phi V(\mu_i)$.



The score equation to be solved for the MLE $\hat{\beta}$ is

$$\sum_{i=1}^{n} \frac{y_i - \hat{\mu}_i}{V(\hat{\mu}_i)} \frac{1}{g'(\hat{\mu}_i)} \mathbf{x}_i = \mathbf{0}$$

which doesn't depend on ϕ and where $g(\hat{\mu}_i) = \mathbf{x}_i^{\top} \hat{\boldsymbol{\beta}}$. Notice, if a canonical link $(g(\mu) = \theta)$ is used, we have

$$g'(\mu) = \frac{\partial \theta}{\partial \mu} = \frac{1}{\partial \mu / \partial \theta} = \frac{1}{\partial b'(\theta) / \partial \theta} = \frac{1}{b''(\theta)} = \frac{1}{V(\mu)}$$

and the above score equation simplifies to

$$\sum_{i=1}^n (y_i - \hat{\mu}_i) \mathbf{x}_i = \mathbf{0}$$

A general method to solve the score equation is the iterative algorithm **Fisher's Method of Scoring** (derived from a Taylor expansion of $s(\beta)$).

In the *t*-th iteration, the new estimate $\boldsymbol{\beta}^{(t+1)}$ is obtained from the previous one $\boldsymbol{\beta}^{(t)}$ by

$$\boldsymbol{\beta}^{(t+1)} = \boldsymbol{\beta}^{(t)} + s(\boldsymbol{\beta}^{(t)}) \left[E\left(\frac{\partial s(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}}\right) \Big|_{\boldsymbol{\beta} = \boldsymbol{\beta}^{(t)}} \right]^{-1}$$

Therefore, the speciality is the usage of the **expected** instead of the **observed** Hessian matrix.

It could be shown that this iteration can be rewritten as

$$\boldsymbol{\beta}^{(t+1)} = \left(\mathbf{X}^{\top}\mathbf{W}^{(t)}\mathbf{X}\right)^{-1}\mathbf{X}^{\top}\mathbf{W}^{(t)}\mathbf{z}^{(t)}$$

with the vector of pseudo-observations $\mathbf{z} = (z_1, \dots, z_n)^{\top}$ and diagonal weight matrix \mathbf{W} defined as

$$z_{i} = g(\mu_{i}) + g'(\mu_{i})(y_{i} - \mu_{i})$$

$$w_{i} = \frac{1}{V(\mu_{i})(g'(\mu_{i}))^{2}}$$

Since

$$\boldsymbol{\beta}^{(t+1)} = \left(\mathbf{X}^{\top}\mathbf{W}^{(t)}\mathbf{X}\right)^{-1}\mathbf{X}^{\top}\mathbf{W}^{(t)}\mathbf{z}^{(t)}$$

the estimate $\hat{\beta}$ is calculated using an **Iteratively (Re-)Weighted Least Squares** (IWLS) algorithm:

- **1** start with initial guesses $\mu_i^{(0)}$ (e.g. $\mu_i^{(0)} = y_i$ or $\mu_i^{(0)} = y_i + c$)
- **2** calculate working responses $z_i^{(t)}$ and weights $w_i^{(t)}$
- $oldsymbol{3}$ calculate $oldsymbol{eta}^{(t+1)}$ by weighted least squares
- 4 repeat steps 2 and 3 till convergence.

Introduction to GLM's: Standard errors

For the MLE $\hat{oldsymbol{eta}}$ it holds that (asymptotically)

$$\hat{oldsymbol{eta}} \sim \mathsf{Normal}(oldsymbol{eta}, \phi(\mathbf{X}^{ op}\mathbf{W}\mathbf{X})^{-1})$$

Thus, standard errors of the estimators $\hat{\beta}_j$ are the respective diagonal elements of the estimated variance/covariance matrix

$$\widehat{\operatorname{var}(\!\hat{oldsymbol{eta}})} = \phi(\mathbf{X}^{ op} \hat{\mathbf{W}} \mathbf{X})^{-1}$$

with $\hat{\mathbf{W}} = \mathbf{W}(\hat{\boldsymbol{\mu}})$. Note that $(\mathbf{X}^{\top}\hat{\mathbf{W}}\mathbf{X})^{-1}$ is a by-product of the last IWLS iteration. If ϕ is unknown, an estimator is required.

Introduction to GLM's: Dispersion estimator

There are practical difficulties when estimating ϕ by ML.

A **method-of-moments** like estimator is developed considering the ratios

$$\phi = \frac{\mathsf{E}(y_i - \mu_i)^2}{V(\mu_i)}$$
, for all $i = 1, \dots, n$

Averaging over all these ratios and assuming that the μ_i 's are known results in the estimator

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

However, since β is unknown we better use the bias-corrected version (also known as the mean generalized Pearson's chi-square statistic)

$$\hat{\phi} = \frac{1}{n-p} \sum_{i=1}^{n} \frac{(y_i - \hat{\mu}_i)^2}{V(\hat{\mu}_i)} = \frac{1}{n-p} X^2$$

The glm Function

Generalized linear models can be fitted in wining the glm function, which is similar to lm for fitting linear models. The arguments to a glm call are as follows:

```
glm(formula, family = gaussian, data, weights, subset,
  na.action, start = NULL, etastart, mustart, offset,
  control = glm.control(...), model = TRUE,
  method = "glm.fit", x = FALSE, y = TRUE,
  contrasts = NULL, ...)
```

The glm Function

Formula argument:

The formula is specified for a glm as e.g.

$$y \sim x1 + x2$$

where x1 and x2 are the names of

- numeric vectors (continuous predictors)
- factors (categorial predictors)

All the variables used in the formula must be in the workspace or in the data frame passed to the data argument.

The glm Function

Formula argument:

Other symbols that can be used in the formula are:

- a:b for the interaction between a and b
- a*b which expands to 1 + a + b + a:b
- . first order terms of all variables in data
- to exclude a term (or terms)
- 1 intercept (default)
- -1 without intercept

The glm Function

Family argument:

The family argument defines the response distribution (variance function) and the **link** function. The exponential family functions available in \mathfrak{Q} are e.g.

- gaussian(link = "identity")
- binomial(link = "logit")
- poisson(link = "log")
- Gamma(link = "inverse")

The glm Function

Extractor functions:

The glm function returns an object of class c("glm", "lm"). There are several methods available to access or display components of a glm object, e.g.

- residuals()
- fitted()
- predict()
- coef()
- deviance()
- summary()
- plot()

The glm Function: Example

temp

```
Refit life expectancies model using glm().
The first part contains the same information as from lm()
> mod <- glm(life.exp ~ urban + log(physicians) + temp)</pre>
> summary(mod)
Call:
glm(formula = life.exp ~ urban + log(physicians) + temp)
Deviance Residuals:
              1Q Median
    Min
                                 3Q
                                          Max
-20.4925 -2.6337 0.7898 3.3447 10.4813
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) 67.37488 1.85916 36.239 < 2e-16 ***
       8.13713 2.59353 3.137 0.00211 **
urban
log(physicians) 3.50002 0.40578 8.625 2.01e-14 ***
```

-0.05590 0.06242 -0.895 0.37219

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The glm Function: Example

Since the default family="gaussian", deviance residuals corresponds to ordinary residuals as in a linear model.

A five-number summary of those raw residuals is given.

Wald tests

Remember that for the MLE it asymptotically holds that

$$\hat{oldsymbol{eta}} \sim \mathsf{Normal}(oldsymbol{eta}, \phi(\mathbf{X}^{ op}\mathbf{W}\mathbf{X})^{-1})$$

Thus, we can utilize this to construct a test statistic on the significance of a coefficient, say β_j for $j=1,\ldots,p-1$. If we test

$$H_0: \beta_j = 0$$
 versus $H_1: \beta_j \neq 0$

we can use the test statistic

$$t = rac{\hat{eta}_j}{\sqrt{\hat{\phi}(\mathbf{X}^{ op}\hat{\mathbf{W}}\mathbf{X})_{j+1,j+1}^{-1}}}$$

which under H_0 asymptotically follows a t distribution with n-p degrees of freedom.



The glm Function: Example

The second part contains some new information on estimated **dispersion** and **goodness-of-fit aspects** which we will discuss later in detail.

First the dispersion estimate (if necessary) $\hat{\phi}$ is provided

(Dispersion parameter for gaussian family taken to be 24.577)

This estimate is simply the squared residual standard error (that was 4.958 in the summary(lm()).

Next there is the **deviance** of two models and the number of missing observations:

```
Null deviance: 10782.0 on 132 degrees of freedom
Residual deviance: 3170.5 on 129 degrees of freedom
(39 observations deleted due to missingness)
```

The first refers to the **null model** which corresponds to a model with intercept only (the iid assumption, no explanatory variables). The associated degrees of freedom are n-1.

The second refers to our **fitted model** with p-1 explanatory variables in the predictor and, thus, with associated degrees of freedom n-p.

The **deviance** of a model is defined as the distance of log-likelihoods, i.e.

$$D(\mathbf{y}, \hat{\boldsymbol{\mu}}) = -2\phi \left(\ell(\hat{\boldsymbol{\mu}}|\mathbf{y}) - \ell(\mathbf{y}|\mathbf{y})\right)$$

Here, $\hat{\mu}$ are the fitted values under the considered model (maximizing the log-likelihood under the given parametrization), and \mathbf{y} denote the estimated means under a model without any restriction at all (thus $\hat{\mu} = \mathbf{y}$ in such a **saturated model**).

For any member of the LEF the deviance equals

$$D(\mathbf{y}, \hat{\boldsymbol{\mu}}) = -2\phi \sum_{i=1}^{n} \frac{(y_i \hat{\theta}_i - y_i \tilde{\theta}_i) - (b(\hat{\theta}_i) - b(\tilde{\theta}_i))}{\phi}$$
$$= -2\sum_{i=1}^{n} \left\{ (y_i \hat{\theta}_i - y_i \tilde{\theta}_i) - (b(\hat{\theta}_i) - b(\tilde{\theta}_i)) \right\}$$

where $\tilde{\theta}_i$ denotes the estimate of θ_i under the saturated model. Under the saturated model, there are as many mean parameters μ_i allowed as observations y_i .

Note that for LEF members the **deviance**

$$D(\mathbf{y}, \hat{\boldsymbol{\mu}}) = -2\sum_{i=1}^{n} \left\{ (y_i \hat{\theta}_i - y_i \tilde{\theta}_i) - (b(\hat{\theta}_i) - b(\tilde{\theta}_i)) \right\}$$

doesn't depend on the dispersion!



Example: Gaussian responses $(\phi = \sigma^2)$ with identity link (LM)

$$\ell(\hat{\boldsymbol{\mu}}|\mathbf{y}) = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2}\sum_{i=1}^{n} \frac{(y_i - \hat{\mu}_i)^2}{\sigma^2}$$
$$\ell(\mathbf{y}|\mathbf{y}) = -\frac{n}{2}\log(2\pi\sigma^2)$$

Therefore the deviance equals the **sum of squared errors**, i.e.

$$D(\mathbf{y}, \hat{\boldsymbol{\mu}}) = -2\phi \left(\ell(\hat{\boldsymbol{\mu}}|\mathbf{y}) - \ell(\mathbf{y}|\mathbf{y})\right) = \sum_{i=1}^{n} (y_i - \hat{\mu}_i)^2 = SSE(\hat{\boldsymbol{\beta}})$$

Finally we have

AIC: 809.22

Number of Fisher Scoring iterations: 2

The **Akaike Information Criterion (AIC)** also assess the fit penalizing for the total number of parameters p+1 (linear predictor and dispersion in this case) and is defined as

$$AIC = -2\ell(\hat{\boldsymbol{\mu}}|\mathbf{y}) + 2(p+1)$$

The smaller the AIC value the better the fit. Use AIC only to compare different models (not necessarily nested). Sometimes, the term $-2\ell(\hat{\mu}|\mathbf{y})$ is called **disparity**.

Residuals

Several different ways to define residuals in a GLM:

- deviance: write deviance as $\sum_{i=1}^{n} d(y_i, \hat{\mu}_i)^2$
- pearson: $r_i^P = (y_i \hat{\mu}_i) / \sqrt{V(\hat{\mu}_i)}$
- working: $r_i^W = \hat{z}_i \hat{\eta}_i = (y_i \hat{\mu}_i)g'(\hat{\mu}_i)$ (remember that $g'(\hat{\mu}_i) = 1/V(\hat{\mu}_i)$ for canonical link models)
- response: $y_i \hat{\mu}_i$
- partial: $r_i^P + \hat{\beta}_j x_{ij}$ is the partial residual for the *j*-th covariate

Except the partial residuals, these types are all equivalent for LM's.

Residuals

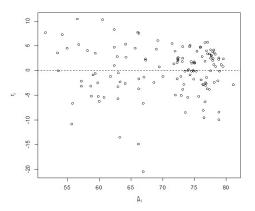
Deviance residuals are the default used in \mathbb{Q} since they reflect the same criterion as used in the fitting.

Plot deviance residuals against fitted values:

```
> plot(residuals(mod) ~ fitted(mod),
+ xlab = expression(hat(mu)[i]),
+ ylab = expression(r[i]))
> abline(0, 0, lty = 2)
```

Residuals

Deviance/Pearson/response/working residuals vs. fitted values:

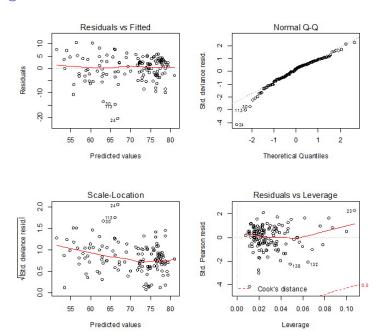


The glm Function: Plot

The plot() function gives the following sequence of plots:

- deviance residuals vs. fitted values
- Normal Q-Q plot of deviance residuals standardized to unit variance
- scale-location plot of standardized deviance residuals
- standardized deviance residuals vs. leverage with Cook's distance contours
- > plot(mod)

The glm Function: Plot



So far we considered (Box-Cox transformation) models like

- $V_i^{1/3} \stackrel{ind}{\sim} \text{Normal}(\mu_i, \sigma^2)$, $E(V^{1/3}) = \mu = H + D$
- $\log(V_i) \stackrel{ind}{\sim} \operatorname{Normal}(\mu_i, \sigma^2)$, $\operatorname{E}(\log(V)) = \mu = \log(H) + \log(D)$

In what follows we will assume that a GLM holds with

• $V_i \stackrel{ind}{\sim} \text{Normal}(\mu_i, \sigma^2) \text{ and } g(\mathsf{E}(V)) = \eta.$

More specifically, we like to check out the models:

- $\mu^{1/3} = H + D$
- $\bullet \log(\mu) = \log(H) + \log(D).$

These models on the **observations scale** can be easily fitted using glm().

```
V_i \stackrel{ind}{\sim} \text{Normal}(\mu_i, \sigma^2), \ \mu^{1/3} = H + D
> pmodel <- glm(V ~ H + D, family = gaussian(link=power(1/3)))</pre>
> summary(pmodel)
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.051322  0.224095  -0.229  0.820518
H
     D
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
(Dispersion parameter for gaussian family taken to be 6.577063)
   Null deviance: 8106.08 on 30 degrees of freedom
Residual deviance: 184.16 on 28 degrees of freedom
```

Number of Fisher Scoring iterations: 4

ATC: 151.21

```
V_i \stackrel{ind}{\sim} \text{Normal}(\mu_i, \sigma^2), \ \mu^{1/3} = H + D
> AIC(pmodel)
[1] 151.2102
> -2*logLik(pmodel) + 2*4
'log Lik.' 151.2102 (df=4)
> logLik(pmodel)
'log Lik.' -71.60508 (df=4)
> sum(log(dnorm(V,pmodel$fit,sqrt(summary(pmodel)$disp*28/31))))
[1] -71.60508
> sum(residuals(pmodel)^2)
[1] 184.1577
> deviance(pmodel)
[1] 184.1577
> sum((V-mean(V))^2) # Null Deviance
[1] 8106.084
```

```
V_i \stackrel{ind}{\sim} \text{Normal}(\mu_i, \sigma^2), \log(\mu) = \log(H) + \log(D)
> summary(glm(V ~ log(H) + log(D), family = gaussian(link=log)))
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -6.53700 0.94352 -6.928 1.57e-07 ***
log(H) 1.08765 0.24216 4.491 0.000111 ***
log(D) 1.99692 0.08208 24.330 < 2e-16 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' '1
(Dispersion parameter for gaussian family taken to be 6.41642)
    Null deviance: 8106.08 on 30 degrees of freedom
Residual deviance: 179.66 on 28 degrees of freedom
```

Number of Fisher Scoring iterations: 4

AIC: 150.44

Gamma responses: $y \sim \text{Gamma}(a, \lambda)$ with density function

$$f(y|a,\lambda) = \exp(-\lambda y)\lambda^a y^{a-1} \frac{1}{\Gamma(a)}, \quad a,\lambda,y>0$$

with
$$E(y) = a/\lambda$$
 and $var(y) = a/\lambda^2$.

Mean parametrization needed!

Reparametrization: define $\mu = \nu/\lambda$, $\nu = a$

$$f(y|a,\lambda) = \exp(-\lambda y)\lambda^{a}y^{a-1}\frac{1}{\Gamma(a)}$$

$$f(y|\mu,\nu) = \exp\left(-\frac{\nu}{\mu}y\right)\left(\frac{\nu}{\mu}\right)^{\nu}y^{\nu-1}\frac{1}{\Gamma(\nu)}$$

$$= \exp\left(\frac{y\left(-\frac{1}{\mu}\right) - \log\mu}{1/\nu} + \nu\log\nu + (\nu-1)\log y - \log\Gamma(\nu)\right)$$

LEF member with:

$$\theta = -1/\mu$$
, $b(\theta) = \log \mu = -\log(-\theta)$, and $\phi = 1/\nu$.



 $Gamma(\mu, \nu)$ belongs to the **LEF** with

$$\theta = -1/\mu$$
, $b(\theta) = \log \mu = -\log(-\theta)$, $\phi = 1/\nu$.

Thus,

$$E(y) = b'(\theta) = -\frac{1}{-\theta} = -\frac{1}{\theta} = \mu$$
$$var(y) = \phi b''(\theta) = \phi \frac{1}{\theta^2} = \phi \mu^2$$

with dispersion $\phi = 1/\nu$ and variance function $V(\mu) = \mu^2$.

Coefficient of variation:

$$\frac{\sqrt{\text{var}(y_i)}}{\mathsf{E}(y_i)} = \frac{\sqrt{\phi\mu_i^2}}{\mu_i} = \sqrt{\phi} = \text{constant for all } i = 1, \dots, n.$$

```
Form of the Gamma(\mu, \nu) density function is determined by \nu.
Functions in \mathbb{Q} are based on shape (=1/\phi) and scale (=\phi\mu)
> y <- (1:400)/100
> shape <- 0.9
> scale <- 1.5
> plot(y, dgamma(y, shape=shape, scale=scale))
> mean(rgamma(10000, shape=shape, scale=scale)); shape*scale
[1] 1.374609
[1] 1.35
> var(rgamma(10000, shape=shape, scale=scale)); shape*(scale)^2
[1] 2.001009
[1] 2.025
```

Gamma distributions are generally **skewed to the right**.

$$\operatorname{shape} < 1 \ (0.9 \ \operatorname{left}) \qquad \operatorname{shape} > 1 \ (1.5 \ \operatorname{right})$$

Special cases: $\nu=1/\phi=1$ (exponential) and $\nu\to\infty$ (normal)

Gamma Regression: Link Function

What's an appropriate link function?

- Canonical link function: $\eta = \theta = -\frac{1}{\mu}$ (inverse-link). Since we need $\mu > 0$ we need $\eta < 0$ giving complicated restriction on $\boldsymbol{\beta}$.
- Thus, the **log-link** is often used without restrictions on η , i.e.

$$\log \mu = \eta$$

Gamma Regression: Deviance

Assume that $y_i \sim \text{Gamma}(\mu_i, \phi)$ (independent) and $\log \mu_i = \eta_i$. Then

$$\ell(\hat{\boldsymbol{\mu}}, \phi | \mathbf{y}) = \sum_{i=1}^{n} \left\{ \frac{y_i \left(-\frac{1}{\hat{\mu}_i} \right) - \log \hat{\mu}_i}{\phi} + c(y_i, \phi) \right\}$$
$$\ell(\mathbf{y}, \phi | \mathbf{y}) = \sum_{i=1}^{n} \left\{ \frac{y_i \left(-\frac{1}{y_i} \right) - \log y_i}{\phi} + c(y_i, \phi) \right\}$$

and thus the scaled deviance equals

$$\frac{1}{\phi}D(\mathbf{y},\hat{\boldsymbol{\mu}}) = -\frac{2}{\phi} \sum_{i=1}^{n} \left\{ \left(-\frac{y_i}{\hat{\mu}_i} - \log \hat{\mu}_i \right) - (-1 - \log y_i) \right\}$$

$$= -\frac{2}{\phi} \sum_{i=1}^{n} \left\{ \log \frac{y_i}{\hat{\mu}_i} - \frac{y_i - \hat{\mu}_i}{\hat{\mu}_i} \right\}$$

Gamma Regression: Dispersion

Method of moments is used to estimate the dispersion parameter. We have a sample y_1, \ldots, y_n with

$$\mathsf{E}(y_i) = \mu_i$$
 and $\mathsf{var}(y_i) = \phi \mu_i^2$, $i = 1, \dots, n$

Consider $z_i = y_i/\mu_i$ with $E(z_i) = 1$ and $var(z_i) = \phi$ (z_i are iid). Thus,

$$\hat{\phi} = \frac{1}{n-p} \sum_{i=1}^{n} \left(\frac{y_i}{\hat{\mu}_i} - 1 \right)^2 = \frac{1}{n-p} \sum_{i=1}^{n} \left(\frac{y_i - \hat{\mu}_i}{\hat{\mu}_i} \right)^2$$

which is equivalent to the mean Pearson statistic.

We now assume that life expectancy follows a **gamma** model.

> gmod <- glm(life.exp ~ urban + log(physicians) + temp,

0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1 ' '1

Given urban and log(physicians) are in the model, temp seems to be **irrelevant** as an additional predictor.

Signif. codes:

The next part of the output contains information about:

(Dispersion parameter for Gamma family taken to be 0.005525322)

The dispersion estimate $\hat{\phi}$ is the mean Pearson statistic

```
> # direct from summary(.)
> summary(gmod)$dispersion
[1] 0.005525322
> # or explicitly calculated as
> sum(residuals(gmod, type="pearson")^2)/gmod$df.resid
[1] 0.005525322
```

giving the estimated response variance as $\widehat{\text{var}}(y_i) = 0.0055 V(\hat{\mu}_i)$.

(Dispersion parameter for Gamma family taken to be 0.005525322)

Null deviance: 2.37804 on 132 degrees of freedom Residual deviance: 0.75412 on 129 degrees of freedom (39 observations deleted due to missingness) ATC: 829.14

AIC: 829.14

Number of Fisher Scoring iterations: 4

For the scaled deviance we get

$$\frac{1}{\hat{\phi}}D(\mathbf{y},\hat{\boldsymbol{\mu}}) = \frac{0.7541}{0.0055} = 136.4838$$

which is pretty close its associated degrees of freedom 129.

Residual Deviance Test:

Model (*): $y_i \stackrel{ind}{\sim} \text{Gamma}(\mu_i = \exp(\eta_i), \phi), i = 1, ..., n.$

Reject model (*) at level α if

$$\frac{1}{\phi}D(\mathbf{y},\hat{\boldsymbol{\mu}}) > \chi^2_{1-\alpha,n-\rho}$$

Since the dispersion ϕ is unknown, we use its estimate $\hat{\phi}$ instead and reject model (*) if

$$\frac{1}{\hat{\phi}}D(\mathbf{y},\hat{\boldsymbol{\mu}})>\chi^2_{1-\alpha,n-p}$$

> 1-pchisq(deviance(gmod)/summary(gmod)\$disp, gmod\$df.resid)
[1] 0.3090557 # p-value

Partial Deviance Test:

Consider the model $g(\boldsymbol{\mu}) = \mathbf{X}_1 \boldsymbol{\beta}_1 + \mathbf{X}_2 \boldsymbol{\beta}_2$ with $\dim(\boldsymbol{\beta}_1) = p_1$, $\dim(\boldsymbol{\beta}_2) = p_2$ and $p = p_1 + p_2$. Now calculate

- $\hat{\boldsymbol{\mu}}_1 = g^{-1}(\mathbf{X}_1\hat{\boldsymbol{\beta}}_1)$: the fitted means under the reduced model with design \mathbf{X}_1 only (corresponds to $H_0: \boldsymbol{\beta}_2 = \mathbf{0}$)
- $\hat{\boldsymbol{\mu}}_2 = g^{-1}(\mathbf{X}_1\hat{\boldsymbol{\beta}}_1 + \mathbf{X}_2\hat{\boldsymbol{\beta}}_2)$: the fitted means under the full model with design \mathbf{X}_1 and \mathbf{X}_2
- $\hat{\phi} = X^2/(n-p)$: dispersion estimate under the full model

Reject H_0 at level α if

$$\frac{\left(D(\mathbf{y},\hat{\boldsymbol{\mu}}_1)-D(\mathbf{y},\hat{\boldsymbol{\mu}}_2)\right)/p_2}{\hat{\boldsymbol{\phi}}} > F_{1-\alpha,p_2,n-p}$$

```
Reject H_0: \beta_{\text{temp}} = 0 if
                \frac{(D(\mathbf{y}, \hat{\boldsymbol{\mu}}_1) - D(\mathbf{y}, \hat{\boldsymbol{\mu}}_2))/1}{\hat{\boldsymbol{\sigma}}} > F_{1-\alpha, 1, n-p}
> (dev2 <- deviance(gmod))</pre>
[1] 0.7541171
> (hatphi <- sum(residuals(gmod, type="pearson")^2)/gmod$df.r)</pre>
[1] 0.005525322
> gmod1 <- glm(life.exp ~ urban + log(physicians),
                   family=Gamma(link="log"))
> (dev1 <- deviance(gmod1))</pre>
[1] 0.7574799
> (F <- ((dev1-dev2)/1)/hatphi)</pre>
[1] 0.6086254
> 1-pf(F, 1, gmod$df.r)
[1] 0.4367349
```

ANalysis Of deViAnce (ANOVA):

Much easier to use again anova():

> anova(gmod, test="F")
Analysis of Deviance Table

Model: Gamma, link: log

Response: life.exp

Terms added sequentially (first to last)

```
Df Deviance Resid. Df Resid. Dev F Pr(>F)

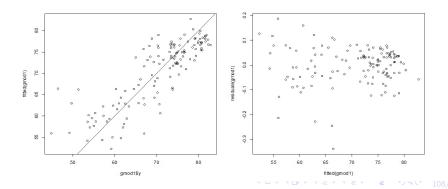
NULL 132 2.37804

urban 1 0.97333 131 1.40471 176.1573 <2e-16 ***
log(phy) 1 0.64723 130 0.75748 117.1394 <2e-16 ***
temp 1 0.00336 129 0.75412 0.6086 0.4367
```

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Some Diagnostic Plots:

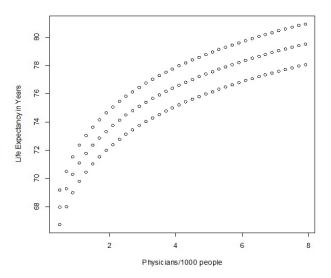
- > plot(gmod1\$y, fitted(gmod1), xlim=c(45,85), ylim=c(45,85))
 > abline(0,1)
- > plot(fitted(gmod1), residuals(gmod1))



Something about the usage of predict()

- newdata: data frame with predictor values for which to predict.
- type: default is on the scale of the linear predictors. The "terms" option returns a matrix giving the fitted values of each term in the model formula on the linear predictor scale.
- se.fit: logical indicator if standard errors are required.
- dispersion: parameter value used in computing standard errors (if omitted, that returned by summary).

Predict life expectancy for urbanization rates of 37, 56, and 74 % (the empirical 25, 50, and 75 % data quartiles).



Remarks about other predictions:

```
> # predict linear predictor \hat\eta_i
> pl <- predict(gmod1, newdata=new, type="link")</pre>
                  3 ...
4.200571 4.219713 4.234009 ....
> # predict each term in the linear predictor separately
> pt <- predict(gmod1, newdata=new, type="terms")</pre>
       urban log(physicians)
1 -0.01974301 -0.028860925
2 -0.01974301 -0.009719531
3 -0.01974301 0.004577365
attr(,"constant")
[1] 4.249175
> attr(pt, "const") + pt[ ,"urban"] + pt[ ,"log(physicians)"]
4.200571 4.219713 4.234009 ...
```

Logistic Regression

Response Variables y_i , i = 1, ..., n:

- **ungrouped**: each variable y_i can take one of two values, say success/failure (or 0/1),
- **grouped**: the variable $m_i y_i$ is the number of successes in a given number of m_i trials; y_i is the **relative** success frequency, $m_i y_i$ denotes the **absolute** success frequency.

Both situations correspond to a **Binomial** (m_i, π_i) model, where in the ungrouped case we have $m_i = 1$.

Question: Is the binomial distribution also a member of the **linear exponential family (LEF)?**

Logistic Regression: LEF Member

Standardized Binomial: $my \sim \text{Binomial}(m, \pi)$ (m known)

$$f(y|m,\pi) = \Pr(Y = y) = \Pr(mY = my) = \binom{m}{my} \pi^{my} (1-\pi)^{m-my}$$

$$= \exp\left(\log\binom{m}{my} + my \log \pi + m(1-y) \log(1-\pi)\right)$$

$$= \exp\left(\frac{y \log \frac{\pi}{1-\pi} - \log \frac{1}{1-\pi}}{1/m} + \log\binom{m}{my}\right), \quad y = 0, \frac{1}{m}, \frac{2}{m}, \dots, 1.$$

If m is another unknown parameter, this is no longer a LEF member!

Logistic Regression: LEF Member

Standardized Binomial: $my \sim \text{Binomial}(m, \pi)$ (m known)

$$f(y|m,\pi) = \exp\left(\frac{y\log\frac{\pi}{1-\pi} - \log\frac{1}{1-\pi}}{1/m} + \log\binom{m}{my}\right), \quad y = 0, \frac{1}{m}, \frac{2}{m}, \dots, 1.$$

Let $\theta = \log \frac{\pi}{1-\pi}$, $(\pi = e^{\theta}/(1+e^{\theta}))$ and $\phi = 1$ then we have identified another LEF member with

$$a = \frac{1}{m}$$
, $b(\theta) = \log \frac{1}{1-\pi} = \log(1+\exp(\theta))$, $c(y,\phi) = \log {m \choose my}$.

Notice: the **dispersion** parameter $\phi = 1$ is **known** in this case and a = 1/m is a **weight** and considered to be **fixed**!

For a sample $m_i y_i \stackrel{ind}{\sim} \text{Binomial}(m_i, \pi_i)$, $y_i = 0, 1/m_i, \dots, 1$, we have $\text{E}(m_i y_i) = m_i \pi_i$ and $\text{var}(m_i y_i) = m_i \pi_i (1 - \pi_i)$ and thus

$$\mathsf{E}(y_i) = \pi_i =: \mu_i \qquad \text{and} \qquad \mathsf{var}(y_i) = \frac{1}{m_i} \mu_i (1 - \mu_i)$$

with restriction $0 < \mu_i < 1$.

Canonical link $g(\mu_i) = b'^{-1}(\mu_i) = \theta_i$ is the **logit link**

$$\operatorname{logit}(\mu_i) = \operatorname{log} \frac{\mu_i}{1 - \mu_i} = \operatorname{log} \frac{m_i \mu_i}{m_i - m_i \mu_i} = \theta_i = \eta_i$$

$$\Rightarrow \mu_i = \frac{\exp(\eta_i)}{1 + \exp(\eta_i)}$$
.

However, in principal any inverse of a continuous distribution function can be used as $g(\cdot)$.

The name **logit** refers to the distribution function of a logistic distributed random variable with density function

$$f(y|\mu,\tau) = \frac{\exp((y-\mu)/\tau)}{\tau\Big(1+\exp((y-\mu)/\tau)\Big)^2}, \qquad \mu \in \mathbb{R}, \ \tau > 0,$$

for which $E(y) = \mu$ and $var(y) = \tau^2 \pi^2/3$ holds.

The density and the cdf of its standard form ($\mu=0,\, au=1$) is

$$f(y|0,1) = \frac{\exp(y)}{(1 + \exp(y))^2}, \quad \mu \in \mathbb{R}, \qquad F(y|0,1) = \frac{\exp(y)}{1 + \exp(y)}$$

for which E(y) = 0 and $var(y) = \pi^2/3$ holds.

F(y|0,1) corresponds to the inverse logit link.



With $g^{-1}(\eta) = \Phi(\eta)$ we refer to a **probit model**. Logit- and probit link are both **symmetric** links.

Extreme value distribution:

Maximum

$$F_{max}(y) = \exp(-\exp(-y)), \qquad y \in \mathbb{R}$$

with $E(y) = \gamma$ (Euler constant $\gamma = 0.577216$) and $var(y) = \pi^2/6$. The inverse of $F_{max}(\cdot)$ results in the **log-log link** and equals

$$g(\mu) = -\log(-\log(\mu)).$$

Minimum

$$F_{min}(y) = 1 - F_{max}(-y) = 1 - \exp(-\exp(y)), \qquad y \in \mathbb{R}$$

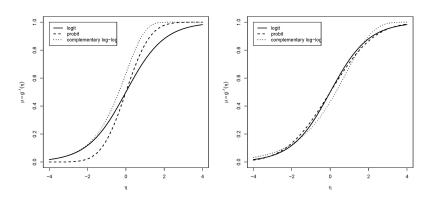
with $E(y) = -\gamma$ and $var(y) = \pi^2/6$.

The inverse of $F_{min}(\cdot)$ is called **complementary log-log link** and equals $g(\mu) = \log(-\log(1-\mu))$.

Both extreme value distribution functions give asymmetric links.

R allows for family=binomial to use several specifications of the link function: logit, probit, cauchit, as also log and cloglog.

```
> euler <- 0.577216
> mu.logit <-function(eta) 1/(1 + exp(-eta))
> mu.probit <-function(eta) pnorm(eta, 0, pi/sqrt(3))</pre>
> mu.cloglog<-function(eta) 1-exp(-exp(-euler+eta/sqrt(2)))
> plot(mu.logit, (-4): 4, xlim = c(-4, 4), ylim = c(0,1),
      xlab = expression(eta),
      ylab = expression(mu == g^-1 * (eta)), lwd=2)
> curve(mu.probit, (-4):4, add = TRUE, lty = 2, lwd=2)
> curve(mu.cloglog, (-4):4, add = TRUE, lty = 3, lwd=2)
> legend(-4, 1, c("logit", "probit", "complementary log-log"),
+ ltv = 1:3, lwd=2)
```



Logistic Regression: Deviance

For $m_i y_i \sim \text{Binomial}(m_i, \mu_i)$ (m_i known) we write the ith log-likelihood contribution as

$$\log f(y_i|m_i, \mu_i) = m_i y_i \log \frac{\mu_i}{1 - \mu_i} - m_i \log \frac{1}{1 - \mu_i} + \log \binom{m_i}{m_i y_i}$$

to get the sample (model and saturated) log-likelihood functions

$$\ell(\hat{\boldsymbol{\mu}}|\mathbf{y}) = \sum_{i=1}^{n} \left\{ m_i y_i \log \frac{\hat{\mu}_i}{1 - \hat{\mu}_i} - m_i \log \frac{1}{1 - \hat{\mu}_i} + \log \binom{m_i}{m_i y_i} \right\}$$

$$\ell(\mathbf{y}|\mathbf{y}) = \sum_{i=1}^{n} \left\{ m_i y_i \log \frac{y_i}{1 - y_i} - m_i \log \frac{1}{1 - y_i} + \log \binom{m_i}{m_i y_i} \right\}.$$

Logistic Regression: Deviance

$$\ell(\hat{\boldsymbol{\mu}}|\mathbf{y}) = \sum_{i=1}^{n} \left\{ m_i y_i \log \frac{\hat{\mu}_i}{1 - \hat{\mu}_i} - m_i \log \frac{1}{1 - \hat{\mu}_i} + \log \binom{m_i}{m_i y_i} \right\}$$

$$\ell(\mathbf{y}|\mathbf{y}) = \sum_{i=1}^{n} \left\{ m_i y_i \log \frac{y_i}{1 - y_i} - m_i \log \frac{1}{1 - y_i} + \log \binom{m_i}{m_i y_i} \right\}.$$

Because of $\phi = 1$ and $a_i = 1/m_i$ the resulting (scaled) deviance is

$$\frac{1}{\phi}D(\mathbf{y}, \hat{\boldsymbol{\mu}}) = -2\sum_{i=1}^{n} \left\{ m_{i}y_{i} \left(\log \frac{\hat{\mu}_{i}}{y_{i}} + \log \frac{1 - y_{i}}{1 - \hat{\mu}_{i}} \right) - m_{i} \log \frac{1 - y_{i}}{1 - \hat{\mu}_{i}} \right\}
= 2\sum_{i=1}^{n} m_{i} \left\{ (1 - y_{i}) \log \frac{1 - y_{i}}{1 - \hat{\mu}_{i}} + y_{i} \log \frac{y_{i}}{\hat{\mu}_{i}} \right\}.$$

Notice: for $y_i = 0$ or 1 independent of $\hat{\mu}_i$ (because $x \log x = 0$ for x = 0) the respective term in the deviance component disappears.

Logistic Regression: Deviance

For binary data $y_i \in \{0, 1\}$ $(m_i = 1 \text{ for all } i)$ we get

$$\ell(\mu_i|y_i) = \begin{cases} \log(1-\mu_i) & \text{if } y_i = 0, \\ \log\mu_i & \text{if } y_i = 1 \end{cases}$$

and

$$d(y_i, \hat{\mu}_i) = \begin{cases} -2\log(1-\hat{\mu}_i) & \text{if } y_i = 0, \\ -2\log\hat{\mu}_i & \text{if } y_i = 1. \end{cases}$$

The deviance increment $d(y_i, \hat{\mu}_i)$ describes the fraction of a binary response of the maximized sample log-likelihood function

$$\ell(\hat{\boldsymbol{\mu}}|\mathbf{y}) = \sum_{i=1}^{n} \ell(\hat{\mu}_i|y_i) = -\frac{1}{2} \sum_{i=1}^{n} d(y_i, \hat{\mu}_i).$$

Bioassay: experimental study based on binary responses, e.g. testing the effect of various concentrations in animal experiments.

Number of animals responding is considered as binomial response.

Example: Insecticide applied on groups (**batches**) of insects of known sizes. When applying a low dose to a group, then no insect will probably fall out. If a high dose is given to another group, many insects of this group will die.

If an insect dies or not when receiving a certain dosage depends on the **tolerance** of the animal. Insects with a low tolerance will rather die on a certain dose than any other with a high tolerance.

Assumption: the tolerance U of an insect is a random variable with density f(u). Insects with tolerance $U < d_i$ will die.

Probability that an animal dies when receiving dose d_i is

$$p_i = \Pr(U < d_i) = \int_{-\infty}^{d_i} f(u) du$$
.

If $U \sim \text{Normal}(\mu, \sigma^2)$, then

$$p_i = \Phi\left(\frac{d_i - \mu}{\sigma}\right) .$$

With $\beta_0 = -\mu/\sigma$ and $\beta_1 = 1/\sigma$ this gives

$$p_i = \Phi(\beta_0 + \beta_1 d_i)$$
 or probit $(p_i) = \Phi^{-1}(p_i) = \beta_0 + \beta_1 d_i$,

i.e. a **probit model** for mortality p_i depending on the dose d_i .



If U follows a **logistic** (μ, τ) model then

$$p_i = \Pr(U \le d_i) = \int_{-\infty}^{d_i} \frac{\exp((u - \mu)/\tau)}{\tau \left(1 + \exp((u - \mu)/\tau)\right)^2} du$$
$$= \frac{\exp((d_i - \mu)/\tau)}{1 + \exp((d_i - \mu)/\tau)}.$$

With $\beta_0 = -\mu/\tau$ and $\beta_1 = 1/\tau$ we get

$$p_i = \frac{\exp(\beta_0 + \beta_1 d_i)}{1 + \exp(\beta_0 + \beta_1 d_i)} \quad \text{or} \quad \log \mathsf{it}(p_i) = \beta_0 + \beta_1 d_i$$

giving a **logistic link model** for p_i .

Example: Effect of poisson given to the *Tobacco Budworm*. Groups of 20 moths of both sex are exposed to various doses of a poisson and the number of killed animals has been recorded.





	Dose in μ g								
sex	1	2	4	8	16	32			
male	1	4	9	13	18	20			
female	0	2	6	10	12	16			

Doses are powers of 2. Thus, we use $log_2(dose)$ as predictor variable.

```
> (ldose <- rep(0:5, 2))
[1] 0 1 2 3 4 5 0 1 2 3 4 5
> (sex <- factor(rep(c("M", "F"), c(6, 6))))
[1] M M M M M M F F F F F
Levels: F M
> (dead <- c(1,4,9,13,18,20,0,2,6,10,12,16))
[1] 1 4 9 13 18 20 0 2 6 10 12 16</pre>
```

- Specification of binomial responses in R by means of a matrix SF (success/failure), in which the **first** (second) column contains the number of **successes** (failures).
- Model describes the **probability of success** (the number of killed animals in our case) at a certain dosage.

```
> summary(budworm.lg <- glm(SF ~ sex*ldose, family = binomial))</pre>
Coefficients:
          Estimate Std. Error z value Pr(>|z|)
(Intercept) -2.9935 0.5527 -5.416 6.09e-08 ***
sexM 0.1750 0.7783 0.225 0.822
ldose 0.9060 0.1671 5.422 5.89e-08 ***
sexM:ldose 0.3529 0.2700 1.307 0.191
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 124.8756 on 11 degrees of freedom
```

Residual deviance: 4.9937 on 8 degrees of freedom

AIC: 43.104

> summary(budworm.lg <- glm(SF ~ sex*ldose, family = binomial))

Here, sex*ldose expands to 1 + sex + ldose + sex:ldose

Thus, it specifies sex-specific submodels of the form:

If sex=female: $\eta = \beta_0 + \beta_{\text{Idose}} \\ \text{Idose}$ If sex=male: $\eta = \left(\beta_0 + \beta_{\text{sexM}}\right) + \left(\beta_{\text{Idose}} + \beta_{\text{sexM:Idose}}\right) \\ \text{Idose}$

Therefore, this interaction term in the model additionally allows for **sex-specific slopes**.

Alternative model specification by numerical vector with elements s_i/a_i , where a_i is the number of trials and s_i the number of successes. The values a_i are specified using weights.

```
> summary(glm(dead/20 ~ sex*ldose, family = binomial,
+ weights=rep(20,12)))
```

Coefficients:

Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1

Result indicates a **significant slope** of ldose for females.

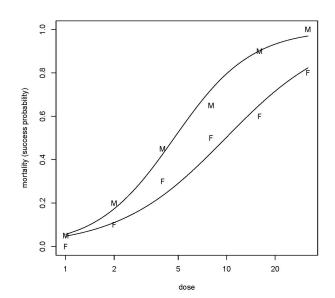
sexM:ldose represents (not significant) a larger slope for males.

First level of sex relates to female moths ("F" before "M") described by the intercept.

sexM is the (not significant) difference of the sex-specific intercepts.

```
> plot(c(1,32), c(0,1), type="n", xlab="dose", log="x")
```

- > text(2^ldose, dead/20, as.character(sex))
- > ld <- seq(0, 5, 0.1), l <- length(ld)
- > lines(2^ld, predict(budworm.lg, data.frame(ldose=ld,
- + sex=factor(rep("M",1,levels=levels(sex))),type="response"))
- > lines(2^ld, predict(budworm.lg, data.frame(ldose=ld,
- + sex=factor(rep("F",1,levels=levels(sex))),type="response"))



sexM describes the difference at dose $1\mu g$ ($log_2(Dose) = 0$) and seems to be irrelevant.

If we are interested in difference at dose $8\mu g$ ($\log_2(Dose) = 3$), we get

```
> summary(budworm.lg8 <- update(budworm.lg, .~sex*I(ldose-3)))
```

Coefficients:

```
Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.2754 0.2305 -1.195 0.23215
sexM 1.2337 0.3770 3.273 0.00107 **
I(ldose - 3) 0.9060 0.1671 5.422 5.89e-08 ***
sexM:I(ldose - 3) 0.3529 0.2700 1.307 0.19117
```

Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1

```
> anova(budworm.lg, test = "Chisq")
```

Significant sex-difference at dose $8\mu g$. Model fits nicely (deviance 5 at df = 8). Confirmed by the analysis of deviance. We resign interactions.

Quadratic 1dose term not necessary.

```
> anova(update(budworm.lg, .~.+ sex*I(ldose^2)), test="Chisq")
```

	Df	Deviance H	Resid. Df	Resid. Dev	Pr(>Chi)	
NULL			11	124.876		
sex	1	6.077	10	118.799	0.0137	*
ldose	1	112.042	9	6.757	<2e-16	***
I(ldose^2)	1	0.907	8	5.851	0.3410	
sex:ldose	1	1.240	7	4.611	0.2655	
<pre>sex:I(ldose^2)</pre>	1	1.439	6	3.172	0.2303	
Signif. codes:	0	'***' 0.00	01 '**' 0	.01 '*' 0.05	5 '.' 0.1	' ' 1

Analysis recommends a model with 2 parallel lines on the predictor- (logit)-axis (1 for each sex).

Estimate dose that guarantees a certain mortality: first reparameterize model, such that each sex has its own intercept.

```
Null deviance: 126.2269 on 12 degrees of freedom Residual deviance: 6.7571 on 9 degrees of freedom
```

AIC: 42.867

 ξ_p is the value of $\log_2(\text{dose})$ inducing mortality p.

 $2^{\xi_{0.5}}$ is the **50% lethal dose** (**LD50**) and using a link $g(p)=\beta_0+\beta_1\xi_p$ we get

$$\xi_p = \frac{g(p) - \beta_0}{\beta_1} \, .$$

Dose ξ_p depends on $\boldsymbol{\beta} = (\beta_0, \beta_1)^{\top}$, thus $\xi_p = \xi_p(\boldsymbol{\beta})$.

Replace β by $\hat{\beta}$ yields estimator $\hat{\xi}_p = \xi_p(\hat{\beta})$ with property (linear approximation)

$$\hat{\xi}_{p}pprox \xi_{p}+(\hat{oldsymbol{eta}}-oldsymbol{eta})^{ op}rac{\partial \xi_{p}(oldsymbol{eta})}{\partial oldsymbol{eta}}$$
 .

Because $\mathsf{E}(\hat{\boldsymbol{\beta}}) \approx \boldsymbol{\beta}$, we have $\mathsf{E}(\hat{\xi}_p) \approx \xi_p$.

Moreover, the delta method gives

$$\operatorname{var}(\hat{\xi}_p) = rac{\partial \xi_p(oldsymbol{eta})}{\partial oldsymbol{eta}^{ op}} \operatorname{var}(\hat{oldsymbol{eta}}) rac{\partial \xi_p(oldsymbol{eta})}{\partial oldsymbol{eta}}$$
 ,

where

$$\frac{\partial \xi_p}{\partial \beta_0} = -\frac{1}{\beta_1}, \qquad \frac{\partial \xi_p}{\partial \beta_1} = -\frac{g(p) - \beta_0}{\beta_1^2} = -\frac{\xi_p}{\beta_1}.$$

Function dose.p from MASS gives for **female** moths:

For **male** moths we get:

An estimated dose of $\log_2(\text{dose}) = 3.264$, or dose = 9.60, is necessary to kill 50% of the female moths, but only dose = 4.69 for 50% of the male moths.

Alternative probit model: gives very similar results.

```
E.g., for female moths we get
```

Logistic Regression: Parameter Interpretation

Assume that the mean of a binary response depends on a two-level factor $x \in \{0, 1\}$.

Cell probabilities:

For x = 1, the **odds** that y = 1 occurs and not y = 0 is

$$\pi_1/(1-\pi_1)$$
.

Its log-transformation

$$\log \frac{\pi_1}{1-\pi_1} = \operatorname{logit}(\pi_1)$$

is called **log-odds** or **Logit**.

The ratio of the odds for x = 1 and the one for x = 0 is called **odds-ratio**

$$\psi = rac{\pi_1/(1-\pi_1)}{\pi_0/(1-\pi_0)}$$
 ,

Its log-transformation is the **log-odds ratio** or the **logit difference**

$$\log \psi = \log \frac{\pi_1/(1-\pi_1)}{\pi_0/(1-\pi_0)} = \operatorname{logit}(\pi_1) - \operatorname{logit}(\pi_0).$$

Let $\mu(x) = \Pr(y = 1|x)$ and $1 - \mu(x) = \Pr(y = 0|x)$, $x \in \{0, 1\}$. The model

$$\log \frac{\mu(x)}{1 - \mu(x)} = \beta_0 + \beta_1 x$$

gives probabilities

As log-odds ratio we get

$$\log \psi = \log \frac{\mu(1)/(1-\mu(1))}{\mu(0)/(1-\mu(0))} = \log \frac{\exp(\beta_0+\beta_1)}{\exp(\beta_0)} = \beta_1.$$

For a general predictor x with a respective model, the odds are

$$\frac{\Pr(y = 1|x)}{\Pr(y = 0|x)} = \frac{\mu(x)}{1 - \mu(x)} = \exp(\beta_0 + \beta_1 x) = \exp(\beta_0) \exp(\beta_1)^x.$$

Interpretation: for a unit change in x, the odds of y = 1 multiply by $\exp(\beta_1)$.

Remission Example: Injection treatment of 27 cancer patients should decay the carcinoma. The response measures whether a patient achieved remission.

Most important explanatory variable LI (labeling index) describes the cell activity after treatment.

For n = 14 different LI values, the response $m_i y_i$ is the number of successful remissions at m_i patients all with labeling index LI_i:

\mathtt{LI}_i	m_i	$m_i y_i$	LI_i	m_i	$m_i y_i$	LI_i	m_i	$m_i y_i$
8	2	0	18	1	1	28	1	1
10	2	0 0	20	3	2	32	1	0
12	3	0	22	2	1	34	1	1
14	3	0	24	1	0	38	3	2
16	3	0	26	1	1			

Assumption: m_i patients in the LI_i group are homogenous, i.e.

$$m_i y_i \stackrel{ind}{\sim} \mathsf{Binomial}(m_i, \mu_i)$$
, with $\log \frac{\mu_i}{1 - \mu_i} = eta_0 + eta_1 \mathsf{LI}_i$.

```
> 1i <- c(seq(8, 28, 2), 32, 34, 38)
```

- > total <-c(2, 2, 3, 3, 3, 1, 3, 2, 1, 1, 1, 1, 1, 3)
- > back <-c(0, 0, 0, 0, 0, 1, 2, 1, 0, 1, 1, 0, 1, 2)
- > SF <- cbind(back, nonback = total back)
- > summary(carcinoma <- glm(SF ~ li, family=binomial))</pre>

Coefficients:

Estimate Std. Error z value Pr(>|z|) (Intercept) -3.7771 1.3786 -2.74 0.0061 ** li 0.1449 0.0593 2.44 0.0146 *

Null deviance: 23.961 on 13 degrees of freedom Residual deviance: 15.662 on 12 degrees of freedom ATC: 24.29

Coefficients:

Interpretation:

- If LI increases by 1 unit, the remission probability multiplies with $\exp(0.145) = 1.156$ (increases by 15.6%).
- Remission prob. is 1/2 if $\hat{\eta} = 0$, i.e. if LI $= -\hat{\beta}_0/\hat{\beta}_1 = 26.07$.
- At the mean LI-value, $\sum_i \text{LI}_i m_i / \sum_i m_i = 20.07$, the linear predictor is $\hat{\beta}_0 + \hat{\beta}_1 20.07 = -0.8691$ (corresponds with 29.54%). There are 9 successes from 27 patients observed, i.e. 33.33%.

Coefficients:

Interpretation:

- Logistic regression curve: $\partial \mu(x)/\partial x = \beta_1 \mu(x)(1 \mu(x))$. Largest ascent in $\mu(x) = 1/2$, i.e. in LI = 26.07, which is $\hat{\beta}_1/4 = 0.0362$.
- \bullet Question: does remission significantly depend on the LI-value? The *p*-value of 1.46% (Wald test) shows evidence for this.

Coefficients:

Null deviance: 23.961 on 13 degrees of freedom Residual deviance: 15.662 on 12 degrees of freedom

AIC: 24.29

Interpretation:

• For an iid random sample model the (NULL) Deviance is 23.96 with df=13. The deviance difference is 8.30 with associated loss of df=1 corresponds to $\chi^2_{1;1-\alpha}$ quantile with $\alpha=0.004$ (even more significant as Wald test).

Significant (positive) association between LI and remission.



Model with each patient remission as **Bernoulli** variable yields the same coefficients, but different values for the deviance and the degrees of freedom.

```
> index <- rep.int(li, times=total)
> B<-c(0,0,0,0,0,0,0,0,0,0,0,0,1,1,1,0,1,0,0,1,1,0,1,1,1,0))
> summary(carcinomaB <- glm(B ~ index, family=binomial))</pre>
```

Coefficients:

```
Estimate Std. Error z value Pr(>|z|) (Intercept) -3.7771 1.3786 -2.74 0.0061 ** index 0.1449 0.0593 2.44 0.0146 *
```

Null deviance: 34.372 on 26 degrees of freedom Residual deviance: 26.073 on 25 degrees of freedom

AIC: 30.07

Again, the deviance difference is the same as before:

```
> anova(carcinomaB, test="Chisq")
```

```
Df Deviance Resid. Df Resid. Dev Pr(>Chi)

NULL 26 34.37

index 1 8.299 25 26.07 0.00397 **

---

Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Notice that the probability of remission (y = 1) is modeled again.

Because all $m_i = 1$ in case of Bernoullis, we do not need to explicitly specify weights.

Binomial responses: relative or absolute **frequencies**.

Poisson responses: counts.

Assumption: mean equals variance, i.e. $E(y_i) = \mu_i = var(y_i)$.

Is the Poisson probability function a member of the linear exponential family (LEF)?

$$y \sim \text{Poisson}(\mu), \ y = 0, 1, 2, ..., \text{ mean } \mu > 0$$
:

$$f(y|\mu) = \frac{\mu^y}{y!}e^{-\mu} = \exp(y\log\mu - \mu - \log y!).$$

Let $\theta = \log \mu$ and $\phi = 1$, then this is a member of the LEF with (weight a = 1)

$$b(\theta) = \exp(\theta)$$
, $c(y, \phi) = -\log y!$.

Canonical link is the **log-link**. **Dispersion** is **known** ($\phi = 1$). Moreover,

$$E(y) = b'(\theta) = \exp(\theta) = \mu$$
$$var(y) = b''(\theta) = \exp(\theta) = \mu.$$

Log-linear model for counts:

$$y_i \stackrel{ind}{\sim} \mathsf{Poisson}(\mu_i)$$
 with $\mathsf{log}(\mu_i) = \eta_i$.

The (scaled) deviance equals $(\phi = 1)$

$$D(\mathbf{y}, \hat{\boldsymbol{\mu}}) = 2\sum_{i=1}^{n} \left\{ y_i \log \frac{y_i}{\hat{\mu}_i} - (y_i - \hat{\mu}_i) \right\}.$$

If the model contains an intercept, this deviance simplifies to

$$D(\mathbf{y}, \hat{\boldsymbol{\mu}}) = 2\sum_{i=1}^{n} y_i \log \frac{y_i}{\hat{\mu}_i}.$$

Deviance contribution is zero for $y_i = 0$ (independent of $\hat{\mu}_i$).

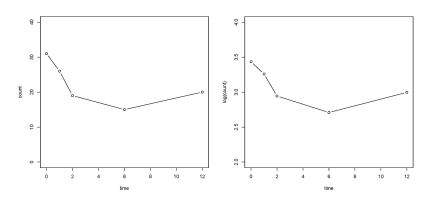
Example: Storing microorganisms (deep-frozen -70° C). Bacterial concentration (counts in a fixed area) measured at initial freezing and then at 1, 2, 6, and 12 months afterwards.

Aim: model from which fractional recovery rates at specified times after freezing can be predicted.

Guess: some sort of exponential decay curve.

- > time <- c(0, 1, 2, 6,12)
 > count <- c(31,26,19,15,20)

 > plot(time, count, type="b", ylim=c(0, 40))
 > plot(time, log(count), type="b", ylim=c(2, 4))



We have expected exponential decay (but last observation is even larger than the two before).

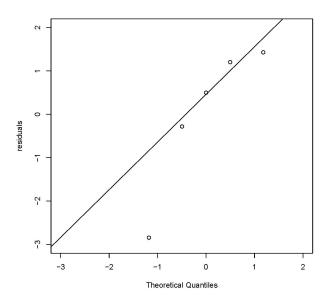
Probably some measurement error causes this behavior.

Possibly log(concentration) depends linearly on time?

Test, if observed curvature is relevant, by allowing the quadratic term time² in the model.

First assumption, counts follow a normal distribution and satisfy a linear model in time and $time^2$.

```
> summary(mo.lm <- lm(count ~ time + I(time^2)))</pre>
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept) 29.80042 1.88294 15.827 0.00397 **
time -4.61601 1.00878 -4.576 0.04459 *
I(time^2) 0.31856 0.08049 3.958 0.05832.
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '1
Residual standard error: 2.438 on 2 degrees of freedom
Multiple R-squared: 0.9252, Adjusted R-squared: 0.8503
F-statistic: 12.36 on 2 and 2 DF, p-value: 0.07483
> gqnorm(residuals(mo.lm), ylab="residuals", xlim=c(-3,2),
+ ylim=c(-3,2), main="")
> qqline(residuals(mo.lm))
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```



Quadratic term seems relevant (p-value 0.058).

Q-Q Plot: points deviate from straight line ⇒ normal assumptions seems unrealistic.

⇒ try Poisson model.

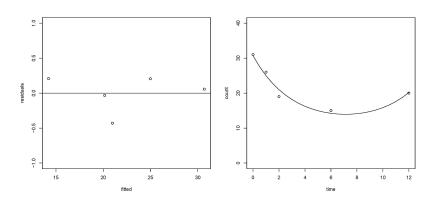
Usually Poisson-means are modeled on log-scale .

Is quadratic time effect still necessary in the model?

```
> summary(mo.P0 <- glm(count ~ time+I(time^2), family=poisson))</pre>
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) 3.423818 0.149027 22.975 <2e-16 ***
time -0.221389 0.095623 -2.315 0.0206 *
I(time^2) 0.015527 0.007731 2.008 0.0446 *
   Null deviance: 7.0672 on 4 degrees of freedom
Residual deviance: 0.2793 on 2 degrees of freedom
AIC: 30.849
> r <- residuals(mo.P0, type="pearson"); sum(r^2)</pre>
[1] 0.2745424
Under true model, deviance (0.2793) and X^2 = 0.2745 should
correspond to about df = n - p = 2 (test on goodness-of-fit).
```

Poisson assumption $(\text{var}(y_i) = \mu_i)$.

Since both values are small, this does not argue against the



Residual plot: if variances equal means, the Pearson residual is

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

If we replace $\hat{\mu}_i$ with μ_i , then r_i should reflect mean zero and variance one.

Residual plot is relatively (n = 5) unremarkable. Poisson assumption seems applicable.

To validate the model quality (exploratively), we plot observed and fitted values against time. Of course, such a 3 parameter model has to fit well the 5 observations.

Measurement errors can also result in growing counts (but this is impossible in reality).

The Wald statistic indicated that $time^2$ seems to be significant in the predictor (p-value 0.0446).

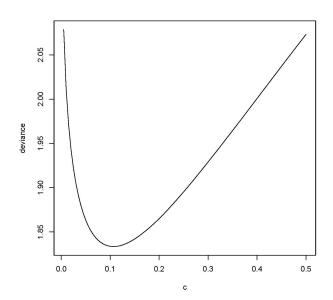
Possibly we get a more realistic model using log(time) instead of time.

If time has a multiplicative effect $(\mu \propto \text{time}^{\gamma})$, then the model should be based on $\log(\text{time})$ as predictor.

But then the starting time log(0) is problematic.

Therefore we consider the transformation log(time + c) with unknown positive shift c.

To determine c, we minimize the deviance in c, i.e.



AIC: 30.403

Optimal value of c under model $1 + \log(\text{time} + c)$ is c = 0.105 and $\log(\text{time} + 0.105)$ will be used from now on as predictor.

```
> time.c <- time + 0.105
> summary(mo.P3 <- glm(count ~ log(time.c), family=poisson))
Coefficients:
          Estimate Std. Error z value Pr(>|z|)
(Intercept) 3.15110 0.09565 32.945 <2e-16 ***
Signif. codes: 0 '***, 0.001 '**, 0.01 '*, 0.05 '., 0.1 ', 1
(Dispersion parameter for poisson family taken to be 1)
   Null deviance: 7.0672 on 4 degrees of freedom
Residual deviance: 1.8335 on 3 degrees of freedom
```

It is again advisable to consider also a model with quadratic time effect in order to check if there is still some curvature left.

Quadratic effect is no longer necessary. It seems that when using the log-transformed shifted time, this linear effect suffices in the predictor.

Wanted: approximative pointwise CIV for $\mu_0 = \exp(\eta_0)$.

Idea 1: use $\hat{\eta}_0 = \mathbf{x}_0^{\top} \hat{\boldsymbol{\beta}}$ with $\widehat{s.e.}(\hat{\eta}_0)$. The transformed 95% interval is

$$CIV(\mu_0) = \left(\exp\left(\hat{\eta}_0 \pm 1.96 \times \widehat{s.e.}(\hat{\eta}_0)\right)\right).$$

Idea 2: Delta method yields

$$\log \hat{\mu} \approx \log \mu + (\hat{\mu} - \mu) \frac{\partial \log \mu}{\partial \mu}$$
,

giving approximative variance, resp. standard error

$$\operatorname{var}(\log \hat{\mu}) \approx \operatorname{var}(\hat{\mu}) \frac{1}{\mu^2}$$

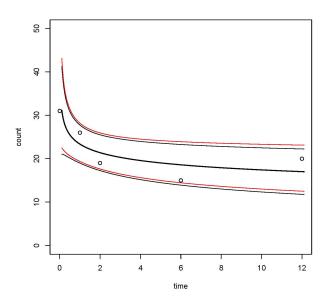
$$\widehat{\operatorname{var}}(\hat{\mu}) \approx \hat{\mu}^2 \operatorname{var}(\hat{\eta}) \qquad \Rightarrow \quad \widehat{s.e.}(\hat{\mu}_0) \approx \hat{\mu}_0 \widehat{s.e.}(\hat{\eta}_0).$$

As 95% CIV we get

$$CIV_{\Delta}(\mu_0) = \left(\hat{\mu}_0 \pm 1.96 \times \hat{\mu}_0 \widehat{\text{s.e.}}(\hat{\eta}_0)\right).$$

```
> # Delta-Method
> t.new <- data.frame(time.c = seq(0,12,.005) + 0.105)
> r.pred<-predict(mo.P3,newdata=t.new,type="response",se.fit=T)</pre>
> fit <- r.pred$fit</pre>
> upper <- fit + qnorm(0.975)*r.pred$se.fit
> lower <- fit - gnorm(0.975)*r.pred$se.fit</pre>
> plot(time, count, type="p", xlab="time", ylab="count")
> lines(time.c.new[,1], upper)
> lines(time.c.new[,1], fit)
> lines(time.c.new[,1], lower)
> # using prediction of type="link"
> l.pred <- predict(mo.P3, newdata=t.new, type="link", se.fit=T)</pre>
> fit <- exp(l.pred$fit)</pre>
> upper <- exp(l.pred$fit + qnorm(0.975)*l.pred$se.fit)</pre>
> lower <- exp(l.pred$fit - gnorm(0.975)*l.pred$se.fit)</pre>
> lines(time.c.new[,1], upper, col=2)
> lines(time.c.new[,1], lower, col=2)

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```



Log-linear models to analyze if 2 factors are **stochastically independent**.

None of the 2 factors will be defined as response – we call them both **classificators**.

Example: Habitat of Lizards: counts on how many lizards have chosen what kind of perch, characterized by two-level factors: height (≥ 4.75 , < 4.75) and diameter (≤ 4.0 , > 4.0). The following counts have been observed:

Perch		diameter			
		≤ 4.0	> 4.0	total	
	≥ 4.75	61	41	102	
height	< 4.75	73	70	143	
total		134	111	245	

Question: are diameter and height classifications independent? Association is measurable by **odds-ratios**. In case of independence, the odds-ratio is 1. We get as estimate

$$\hat{\psi} = \frac{61/41}{73/70} = \frac{61/73}{41/70} = 1.43.$$

Does this indicate that for the true parameter $\psi \neq 1$ holds?

We introduce a log-linear model for 2×2 tables and define the following observed counts:

	В						
Α	1	2	total				
1	<i>y</i> ₁₁	<i>y</i> ₁₂	<i>y</i> _{1•}				
2	<i>y</i> 21	<i>y</i> 21	<i>y</i> _{2•}				
total	<i>y</i> •1	<i>y</i> •2	<i>y</i> ••				

with $y_{\bullet \bullet} = n$, the sample size.

If y_{kl} are Poisson counts and we use a log-link function and A and B as explanatory predictors, this would correspond to a log-linear model.

Distributions of A and of B (marginals) are not of interest.

We consider the next two models

- 1 A + B (independence),
- 2 $A * B \equiv A + B + A : B$ (dependence, saturated model).

Independence Model:

Assumption: for all pairs (a_i, b_i) , i = 1, ..., n, the probability to fall in cell (k, l) is π_{kl} . Then

$$E(y_{kl}) = \mu_{kl} = n \cdot \pi_{kl}, \quad k, l \in \{1, 2\}.$$

In case of stochastic independence, i.e. if

$$\pi_{kl} = \Pr(A = k, B = l) = \Pr(A = k) \Pr(B = l) = \pi_k^A \pi_l^B$$
,

then the associated log-linear model is

$$\log \mu_{kl} = \log n + \log \pi_k^A + \log \pi_l^B.$$

The logarithm of the expected count in cell (k, l) is an additive function of the k-th row effect and the l-th column effect. Thus

$$\log \mu_{kl} = \lambda + \lambda_k^A + \lambda_l^B, \qquad k, l \in \{1, 2\}.$$

$$\log \mu_{kl} = \lambda + \lambda_k^A + \lambda_l^B, \qquad k, l \in \{1, 2\}.$$

How to define the parameters, and how many are identifiable? If a contrast parametrization is of interest, we define

$$\begin{split} \lambda_{k}^{A} &= \log \pi_{k}^{A} - \frac{1}{2} \sum_{h=1}^{2} \log \pi_{h}^{A} \\ \lambda_{l}^{B} &= \log \pi_{l}^{B} - \frac{1}{2} \sum_{h=1}^{2} \log \pi_{h}^{B} \\ \lambda &= \log n + \frac{1}{2} \sum_{h=1}^{2} \log \pi_{h}^{A} + \frac{1}{2} \sum_{h=1}^{2} \log \pi_{h}^{B} \,. \end{split}$$

With this parametrization (deviation from the means) we have

$$\sum_{k=1}^{2} \lambda_{k}^{A} = \sum_{k=1}^{2} \left\{ \log \pi_{k}^{A} - \frac{1}{2} \sum_{h=1}^{2} \log \pi_{h}^{A} \right\} = 0 = \sum_{l=1}^{2} \lambda_{l}^{B}.$$

$$\sum_{k=1}^{2} \lambda_{k}^{A} = \sum_{k=1}^{2} \left\{ \log \pi_{k}^{A} - \frac{1}{2} \sum_{h=1}^{2} \log \pi_{h}^{A} \right\} = 0 = \sum_{l=1}^{2} \lambda_{l}^{B}.$$

Besides λ there is only 1 row and 1 column parameter identifiable. For both others $\lambda_2^A = -\lambda_1^A$, $\lambda_2^B = -\lambda_1^B$ hold.

This model is called log-linear **independence model**. The respective predictors are

Alternative parametrization: **reference cell** instead of contrasts. Characterize an arbitrary cell as reference and define parameters, that describe the deviations from this reference cell.

If e.g. cell (1,1) is the reference, this gives

$$\begin{aligned} \lambda_k^A &= \log \pi_k^A - \log \pi_1^A \\ \lambda_l^B &= \log \pi_l^B - \log \pi_1^B \\ \lambda &= \log n + \log \pi_1^A + \log \pi_1^B \end{aligned}$$

with identifiability constraints

$$\lambda_1^A = \lambda_1^B = 0$$
.

The respective predictors are

		В				
A	1	2				
1	λ	$\lambda + \lambda_2^B$				
2	$\lambda + \lambda_2^A$	$\lambda + \lambda_2^A + \lambda_2^B$				
		< □ > < □ > ·	(불) ←불)	=	200	

Notice that this (reference cell) parametrization results in

$$\log \psi = \log \frac{\mu_{11}/\mu_{12}}{\mu_{21}/\mu_{22}}$$

$$= \log \mu_{11} - \log \mu_{12} - \log \mu_{21} + \log \mu_{22}$$

$$= \lambda - (\lambda + \lambda_2^B) - (\lambda + \lambda_2^A) + (\lambda + \lambda_2^A + \lambda_2^B)$$

$$= 0.$$

Thus, an odds-ratio of $\psi=1$ is equivalent with independence.

This holds independently of the choice of the reference cell.

Saturated (full) Model:

If no independence can be assumed we define

$$\log \mu_{kl} = \lambda + \lambda_k^A + \lambda_l^B + \lambda_{kl}^{AB}, \qquad k, l \in \{1, 2\}.$$

The interaction parameters λ_{kl}^{AB} describe the discrepancies from the independence model.

If contrasts should be used, then the parameters are based on the linear predictors $\eta_{kl} = \log \mu_{kl}$. Let

$$\eta_{k\bullet} = \frac{1}{2} \sum_{l=1}^{2} \eta_{kl}, \quad \eta_{\bullet l} = \frac{1}{2} \sum_{k=1}^{2} \eta_{kl}, \quad \eta_{\bullet \bullet} = \lambda = \frac{1}{2} \frac{1}{2} \sum_{k=1}^{2} \sum_{l=1}^{2} \eta_{kl}.$$

Define row effects λ_k^A , column effects λ_l^B , and interaction effects λ_{kl}^{AB} as deviations from the mean predictor

$$\begin{split} \lambda_k^A &= \eta_{k\bullet} - \eta_{\bullet\bullet} \\ \lambda_l^B &= \eta_{\bullet l} - \eta_{\bullet\bullet} \\ \lambda_{kl}^{AB} &= \eta_{kl} - \eta_{k\bullet} - \eta_{\bullet l} + \eta_{\bullet\bullet} = \underbrace{\left(\eta_{kl} - \eta_{\bullet\bullet}\right)}_{\eta_{kl} - \lambda} - \underbrace{\left(\eta_{k\bullet} - \eta_{\bullet\bullet}\right)}_{\lambda_k^A} - \underbrace{\left(\eta_{\bullet l} - \eta_{\bullet\bullet}\right)}_{\lambda_l^B} \,. \end{split}$$

 λ_k^A , λ_l^B denote deviations from the predictor mean λ . λ_{kl}^{AB} are cell effects that are adjusted for row and column effects. Since all parameters are centered around their means we have

$$\sum_{k=1}^{2} \lambda_{k}^{A} = \sum_{l=1}^{2} \lambda_{l}^{B} = 0.$$

Thus, again only 1 free row and 1 free column parameter.

For the interactions we get

$$\sum_{k=1}^{2} \lambda_{kl}^{AB} = \sum_{k=1}^{2} \eta_{kl} - \sum_{k=1}^{2} \eta_{k\bullet} - 2\eta_{\bullet l} + 2\eta_{\bullet \bullet}$$
$$= 2\eta_{\bullet l} - 2\eta_{\bullet \bullet} - 2\eta_{\bullet l} + 2\eta_{\bullet \bullet} = 0 = \sum_{l=1}^{2} \lambda_{kl}^{AB}.$$

Because of this, the sum of all interactions in each row and in each column is 0.

In case of a 2×2 table there is only 1 free interaction parameter!

The independence model is a special case of the full model with $\lambda_{kl}^{AB} = 0$ for all (k, l).

The additional parameters λ_{kl}^{AB} are **association parameters**, describing the deviations from independence between A and B.

The total number of free parameters is 3 under the independence model and 4 in case of the dependence model.

Default approach in \mathbb{Q} is to use a treatment parametrization, i.e. a reference cell (1,1). If a sum parametrization should be used, then (for *unordered* and *ordered* factors)

```
> options(contrasts=c("contr.sum", "contr.poly"))
```

We can change back to the treatment parametrization through

```
> options(contrasts=c("contr.treatment", "contr.poly"))
```

It's again simpler to work with a reference cell, e.g. cell (1, 1). Setting $\lambda=\eta_{11}$ gives

$$\lambda_{k}^{A} = \eta_{k1} - \eta_{11}$$

$$\lambda_{l}^{B} = \eta_{1l} - \eta_{11}$$

$$\lambda_{kl}^{AB} = \eta_{kl} - \eta_{k1} - \eta_{1l} + \eta_{11} = \underbrace{(\eta_{kl} - \eta_{11})}_{\eta_{kl} - \lambda} - \underbrace{(\eta_{k1} - \eta_{11})}_{\lambda_{k}^{A}} - \underbrace{(\eta_{1l} - \eta_{11})}_{\lambda_{l}^{B}}.$$

Thus $\lambda_1^A = \lambda_1^B = 0$. Moreover all interactions in the first row and in the first column are 0 and we get

What are the MLEs of these parameters?

$$\log \hat{\mu}_{11} = \hat{\lambda} = \log y_{11}$$

$$\log \hat{\mu}_{21} = \hat{\lambda} + \hat{\lambda}_2^A = \log y_{21} \Rightarrow \hat{\lambda}_2^A = \log y_{21} - \log y_{11} = \log \frac{y_{21}}{y_{11}}$$
$$\log \hat{\mu}_{12} = \hat{\lambda} + \hat{\lambda}_2^B = \log y_{12} \Rightarrow \hat{\lambda}_2^B = \log y_{12} - \log y_{11} = \log \frac{y_{12}}{y_{11}}$$

$$\begin{split} \log \hat{\mu}_{22} &= \hat{\lambda} + \hat{\lambda}_2^A + \hat{\lambda}_2^B + \hat{\lambda}_{22}^{AB} = \log y_{22} \\ &\Rightarrow \hat{\lambda}_{22}^{AB} = \log y_{22} - \log y_{11} - \log \frac{y_{21}}{y_{11}} - \log \frac{y_{12}}{y_{11}} = \log \frac{y_{11}y_{22}}{y_{12}y_{21}} \,. \end{split}$$

MLE of the interaction effect is the observed log-odds-ratio, that estimates the deviation from the independence model.

Example: Habitat of Lizards

```
To use cell (1,1) as reference in \mathbb{Q}, we need e.g.
```

```
> count < c(61, 41, 73, 70)
> (hei <- factor(c(">4.75", ">4.75", "<4.75", "<4.75")))</pre>
[1] >4.75 >4.75 <4.75 <4.75
Levels: \langle 4.75 \rangle \langle 4.75 \rangle
> (height <- relevel(hei, ref = ">4.75"))
[1] >4.75 >4.75 <4.75 <4.75
Levels: >4 75 <4 75
> diameter <- factor(c("<4.0", ">4.0", "<4.0", ">4.0"))
```

```
> summary(dep<-glm(count ~ height * diameter, family=poisson))</pre>
```

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)	
(Intercept)	4.1109	0.1280	32.107	<2e-16	***
height<4.75	0.1796	0.1735	1.035	0.3006	
diameter>4.0	-0.3973	0.2019	-1.967	0.0491	*
height<4.75:diameter>4.0	0.3553	0.2622	1.355	0.1754	

```
Null deviance: 1.0904e+01 on 3 degrees of freedom Residual deviance: -8.8818e-16 on 0 degrees of freedom
```

AIC: 31.726

Deviance = 0 on df = 0. Model reproduces the data exactly. Estimated odds-ratio is

Under the independence model we get

```
> summary(ind<-glm(count ~ height + diameter, family=poisson))</pre>
```

Coefficients:

```
Estimate Std. Error z value Pr(>|z|)
(Intercept) 4.0216 0.1148 35.023 < 2e-16 ***
height<4.75 0.3379 0.1296 2.607 0.00913 **
diameter>4.0 -0.1883 0.1283 -1.467 0.14231
```

Null deviance: 10.9036 on 3 degrees of freedom Residual deviance: 1.8477 on 1 degrees of freedom

AIC: 31.574

Odds-ratio is 0 now and the deviance increases by 1.85. This can be used as test statistic on $H_0: \psi = 1$ giving a p-value of

```
> pchisq(ind$deviance, 1, lower.tail = FALSE)
[1] 0.174055
```

Evidence for a non-significant improvement (compare with p-value 0.1754 of the respective Wald statistic). Thus we cannot reject $H_0: \psi=1$ and diameter and height seem to classify independently!

More than two-level factors:

Results can be generalized for **multi-level** classifying factors. Let A be a K-level and B a L-level factor. The **independence model** is

$$\log \mu_{kl} = \lambda + \lambda_k^A + \lambda_l^B, \qquad k = 1, \dots, K, \ l = 1, \dots, L.$$

With cell (1,1) as reference we define

$$\lambda_k^A = \log \pi_k^A - \log \pi_1^A$$
$$\lambda_l^B = \log \pi_l^B - \log \pi_1^B$$
$$\lambda = \log n + \log \pi_1^A + \log \pi_1^B$$

and the same set of identifiability conditions hold, i.e.

$$\lambda_1^A = \lambda_1^B = 0$$
.

There are 1 + (K - 1) + (L - 1) parameter freely estimable. 99.00 = 105/215

Respective predictors are

MLEs are now for
$$k=1,\ldots,K$$
 and $l=1,\ldots,L$
$$\log \hat{\mu}_{11}=\hat{\lambda}=\log \frac{y_{1\bullet}y_{\bullet1}}{y_{\bullet\bullet}}$$

$$\log \hat{\mu}_{k1} = \hat{\lambda} + \hat{\lambda}_k^A = \log \frac{y_{k \bullet} y_{\bullet 1}}{y_{\bullet \bullet}} \Rightarrow \hat{\lambda}_k^A = \log \frac{y_{k \bullet} y_{\bullet 1}}{y_{\bullet \bullet}} - \log \frac{y_{1 \bullet} y_{\bullet 1}}{y_{\bullet \bullet}} = \log \frac{y_{k \bullet}}{y_{1 \bullet}}$$

$$\log \hat{\mu}_{1I} = \hat{\lambda} + \hat{\lambda}_I^B = \log \frac{y_{1\bullet}y_{\bullet I}}{y_{\bullet \bullet}} \Rightarrow \hat{\lambda}_I^B = \log \frac{y_{1\bullet}y_{\bullet I}}{y_{\bullet \bullet}} - \log \frac{y_{1\bullet}y_{\bullet 1}}{y_{\bullet \bullet}} = \log \frac{y_{\bullet I}}{y_{\bullet 1}}$$

The **saturated model** for a $K \times L$ table is

$$\log \mu_{kl} = \lambda + \lambda_k^A + \lambda_l^B + \lambda_{kl}^{AB}, \qquad k = 1, \dots, K, \ l = 1, \dots, L.$$

With reference cell (1, 1) we get for all k = 1, ..., K, l = 1, ..., L

$$\begin{split} \lambda_{k}^{A} &= \eta_{k1} - \eta_{11} \\ \lambda_{l}^{B} &= \eta_{1l} - \eta_{11} \\ \lambda_{kl}^{AB} &= \eta_{kl} - \eta_{k1} - \eta_{1l} + \eta_{11} = \underbrace{(\eta_{kl} - \eta_{11})}_{\eta_{kl} - \lambda} - \underbrace{(\eta_{k1} - \eta_{11})}_{\lambda_{k}^{A}} - \underbrace{(\eta_{1l} - \eta_{11})}_{\lambda_{l}^{B}}, \end{split}$$

where $\lambda_1^A = \lambda_1^B = 0$.

Again, all interactions in row 1 and in column 1 are 0.

Thus, the total number of estimable parameters is $1 + (K - 1) + (L - 1) + (K - 1)(L - 1) = K \times L$.

The predictors are defined as:

Saturated model allows for (K-1)(L-1) additional parameters than the independence model.

Example: Recurrences of Cervical Cancer

Are the predictive factors border zone (BZ) involvement and number affected lymph node (LN) stations classifying independently?

Consider the following counts:

	LN stations			
	0	1	2	≥ 3
BZ not involved	124	21	16	13
BZ involved	58	12	7	5
more than BZ inv.	14	19	12	12

We first fit the saturated model to the data and then test on necessary interactions.

There is evidence, that the 6 interaction parameter are unequal 0 and thus the independence hypothesis can be rejected.

Alternatively, we consider the Pearson statistic under the independence model, i.e.

$$X^{2} = \sum_{i=1}^{3} \sum_{j=1}^{4} \frac{(y_{ij} - \hat{\mu}_{ij})^{2}}{\hat{\mu}_{ij}}$$

with $\log \mu_{ij} = \lambda + \lambda_i^B + \lambda_j^L$. Its realization is

- > ind <- glm(total ~ B+L, family=poisson)</pre>
- > r <- residuals(ind, type="pearson")</pre>
- $> sum(r^2)$
- [1] 43.83645

and equals the χ^2 test statistic in the analysis of contingency tables.

Pearson statistic can be also directly calculated as

```
> (N <- matrix(total, 3, 4, byrow=TRUE))
     [,1] [,2] [,3] [,4]
[1,] 124     21     16     13
[2,]     58     12     7     5
[3,]     14     19     12     12
> chisq.test(N)
```

Pearson's Chi-squared test

```
data: N
X-squared = 43.8365, df = 6, p-value = 7.965e-08
```

Poisson- and binomial distributed responses seem to have some similarities in $K \times 2$ tables.

Denote the table entries by N_{kl} , $k=1,\ldots,K$ and $l\in\{1,2\}$ (e.g. k different experimental environments and l response categories "success l failure").

For independent counts $N_{kl} \stackrel{ind}{\sim} \text{Poisson}(\mu_{kl})$, conditioning on the total number of both responses, say $N_{k\bullet} = N_{k1} + N_{k2}$, results in

$$N_{k2}|N_{k\bullet} \sim \text{Binomial}(N_{k\bullet}, \pi_k), \qquad k = 1, ..., K,$$

with

$$\pi_k = \frac{\mu_{k1}}{\mu_{k1} + \mu_{k2}} \, .$$

Because we assume $N_{k1} \stackrel{ind}{\sim} Poisson(\mu_{k1})$

$$\Pr(N_{k1} = n_{k1}) = \frac{\mu_{k1}^{n_{k1}}}{n_{k1}!} e^{-\mu_{k1}}$$

and thus

$$\Pr(N_{k\bullet} = n_{k\bullet}) = \frac{\mu_{k\bullet}^{n_{k\bullet}}}{n_{k\bullet}!} e^{-\mu_{k\bullet}}$$

with $\mu_{k\bullet} = \mu_{k1} + \mu_{k2}$ and $n_{k\bullet} = n_{k1} + n_{k2}$.

Notice that N_{k1} denoted the number of successes and $N_{k\bullet}$ the total number of trials in the k-th environment.

Given the total number of trials we get conditionally

$$Pr(N_{k1} = n_{k1} | N_{k\bullet} = n_{k\bullet}) = \frac{Pr(N_{k1} = n_{k1}, N_{k2} = n_{k2})}{Pr(N_{k\bullet} = n_{k\bullet})}$$

$$= \frac{\frac{\mu_{k1}^{n_{k1}}}{n_{k1}!} e^{-\mu_{k1}} \frac{\mu_{k2}^{n_{k2}}}{n_{k2}!} e^{-\mu_{k2}}}{\frac{(\mu_{k1} + \mu_{k2})^{n_{k1} + n_{k2}}}{(n_{k1} + n_{k2})!} e^{-(\mu_{k1} + \mu_{k2})}}$$

$$= \frac{(n_{k1} + n_{k2})!}{n_{k1}! n_{k2}!} \frac{\mu_{k1}^{n_{k1}}}{(\mu_{k1} + \mu_{k2})^{n_{k1}}} \frac{\mu_{k2}^{n_{k2}}}{(\mu_{k1} + \mu_{k2})^{n_{k2}}}$$

$$= \binom{n_{k1} + n_{k2}}{n_{k1}} \left(\frac{\mu_{k1}}{\mu_{k1} + \mu_{k2}}\right)^{n_{k1}} \left(\frac{\mu_{k2}}{\mu_{k1} + \mu_{k2}}\right)^{n_{k2}}$$

$$= \binom{n_{k\bullet}}{n_{k1}} \pi_{k1}^{n_{k1}} (1 - \pi_{k})^{n_{k2}}.$$

Moreover, since

$$\operatorname{logit}(\pi_k) = \log \frac{\pi_k}{1 - \pi_k} = \log \frac{\mu_{k1}}{\mu_{k2}} = \log \mu_{k1} - \log \mu_{k2}$$

the logit of the success probability (under the binomial model) is equivalent with an effect on the log-linear axis (under the Poisson model).

Example: Recurrences of Cervical Cancer

Analyse if lymphatic involvement influences the probability of recurrence.

	L = 0	L = 1	L=2	L = 3
R = 0	153	23	12	2
R = 1	43	29	23	28

This can be analyzed either by a log-linear Poisson model or a logistic Binomial model.

```
> count <- c(153, 23, 12, 2, 43, 29, 23, 28)
> L <- factor(c(0, 1, 2, 3, 0, 1, 2, 3))
> R <- c(0, 0, 0, 0, 1, 1, 1, 1)</pre>
```

```
> summary(mod.P <- glm(count ~ R*L + L, family=poisson))</pre>
Coefficients:
          Estimate Std. Error z value Pr(>|z|)
(Intercept) 5.03044 0.08085 62.223 < 2e-16 ***
R.
         -1.26924 0.17260 -7.354 1.93e-13 ***
L1
       -1.89494 0.22364 -8.473 < 2e-16 ***
1.2
        -2.54553 0.29978 -8.491 < 2e-16 ***
L3
          -4.33729 0.71171 -6.094 1.10e-09 ***
R:L1
     1.50104 0.32826 4.573 4.81e-06 ***
R:L2 1.91983 0.39573 4.851 1.23e-06 ***
R:L3
         3.90830 0.75200 5.197 2.02e-07 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '1
```

Null deviance: 3.0017e+02 on 7 degrees of freedom Residual deviance: -4.4409e-15 on 0 degrees of freedom ATC: 55.771

AIC: 55.771

```
> summary(mod.B <- glm(R ~ L, family=binomial, weight=count))
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) -1.2692 0.1726 -7.354 1.93e-13 ***
L1
         1.5010 0.3283 4.573 4.81e-06 ***
1.2
           1.9198 0.3957 4.851 1.23e-06 ***
T.3
          3.9083 0.7520 5.197 2.02e-07 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
   Null deviance: 419.46 on 7 degrees of freedom
```

Residual deviance: 337.34 on 4 degrees of freedom

AIC: 345.34

The specification R*L+L for predictor in log-linear model consists of 2 parts:

- R*L relates on the interaction between binomial R and predictor under the logistic model (L).
- L is saturated with respect of the classifying factor and only ensures that for each of the 4 cell pairs (counts of R=0 and R=1) the observed numbers equal the estimated numbers (reproducing the marginal binomial total sums). Therefore, the interactions with R in the log-linear model (i.e. parameters R, R:L1, R:L2, and R:L3) correspond to the parameters in the logistic model.

This technique can be easily extended for **multinomial** responses.

The linear predictor contains again the sum of 2 parts.

- Specify the cell in which the multinomial observation has been observed (interaction of all classifying factors, L before).
- Specify the interaction (R*(1+L)) between the multinomial category indicator (R) with the considered model (1+L).

However, it is easier to use

- > library(nnet)
- > multinom(formula)

```
> count <- c(rez, total-rez)</pre>
> (R <- gl(2, 12, labels=1:0))
Levels: 1 0
> (L <- factor(rep(rep(0:3, 3), 2)))
[1] 0 1 2 3 0 1 2 3 0 1 2 3 0 1 2 3 0 1 2 3 0 1 2 3
Levels: 0 1 2 3
> (B <- factor(rep(rep(0:2, each=4), 2)))
Levels: 0 1 2
```

ATC: 134.75

```
> summary(MN.glm <- glm(count ~ R*(L+B) + L*B, family=poisson))</pre>
Coefficients:
          Estimate Std. Error z value Pr(>|z|)
          3.032932  0.203404  14.911  < 2e-16 ***
(Intercept)
R.O
         1.604143 0.219202 7.318 2.51e-13 ***
L1
         L2
         -0.870085 0.352170 -2.471 0.013487 *
L3
         -0.573696 0.349225 -1.643 0.100431
B1
         -0.196387 0.286157 -0.686 0.492530
B2
         RO:L1
       -1.287280 0.347971 -3.699 0.000216 ***
R0:L2
        -1.778549
                   0.412032 -4.317 1.59e-05 ***
R0:L3
        -3.797851 0.761597 -4.987 6.14e-07 ***
R0:G1
        -0.728501 0.312710 -2.330 0.019825 *
R0:G2
       Null deviance: 434.130
                      on 23 degrees of freedom
Residual deviance: 10.798
                           degrees of freedom
                      on
```

 4□ → 4□ → 4 ≧ → 4 ≧ → 214/215

Information on observed counts as weights. Same estimates/std.errors as before.