

Generalized Linear Models and Extensions

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Course Outline

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Introduction

- Agricultural Science - different types of data: continuous and discrete.
- Model selection - important part of the research: search for a simple model which explains well the data (Parsimony).
- All models involve:
 - a systematic component - regression, analysis of variance, analysis of covariance;
 - a random component - distributions;
 - a link between systematic and random components.

Motivating examples

Melon organogenesis

	Eldorado				AF-522			
Replicates	0.0	0.1	0.5	1.0	0.0	0.1	0.5	1.0
1	0	0	7	8	0	0	4	7
2	0	2	8	8	0	2	7	8
3	0	0	8	8	0	0	7	8
4	0	1	5	8	0	1	8	8
5	0	0	7	5	0	1	8	7

Considerations

- Response variable: Y – number of explants (cuts of cotyledon) regenerated out of $m = 8$ explants.
- Distribution: Binomial.
- Systematic component: factorial 2×4 (2 varieties, 4 concentrations of BAP(mg/l)), completely randomized tissue culture experiment.
- Aim: to see how organogenesis is affected by variety and concentration of BAP.

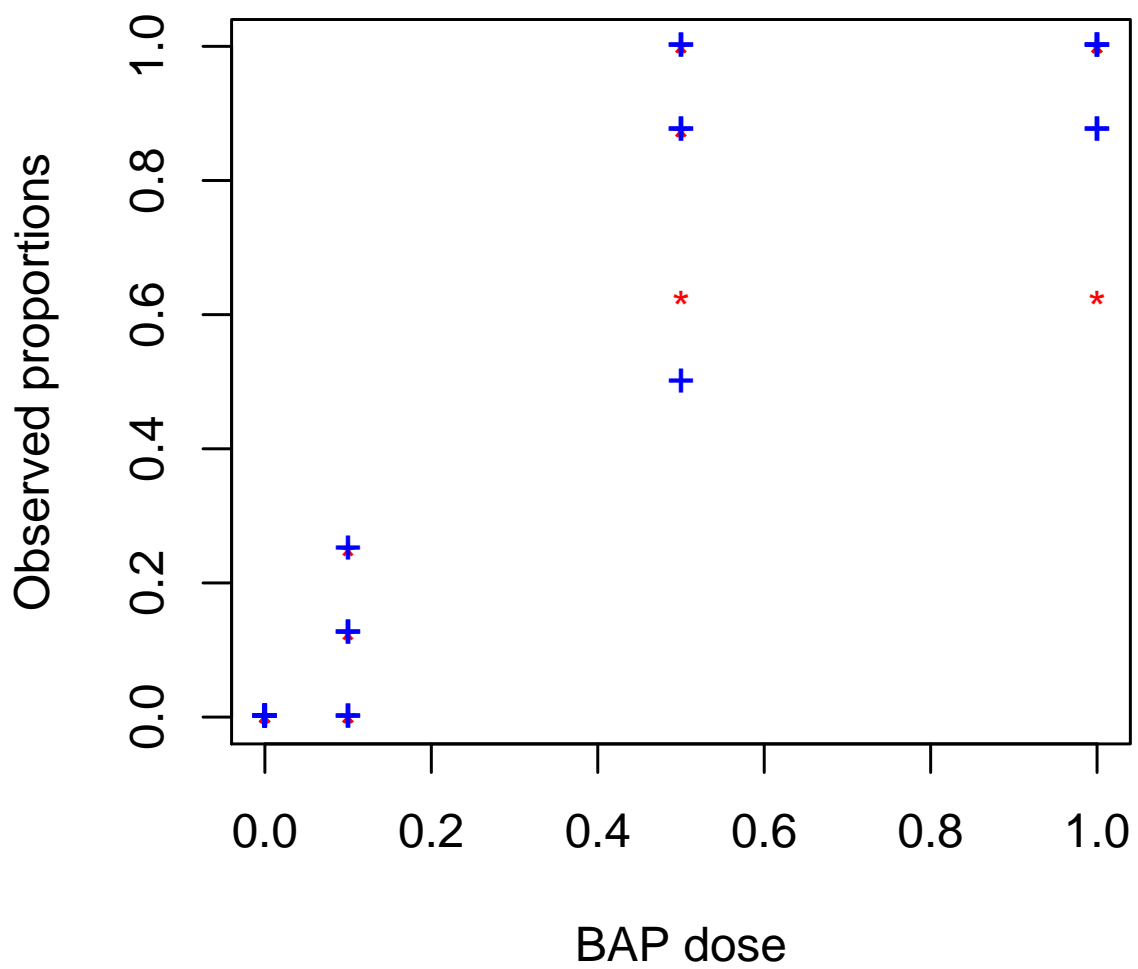


Figure 1. Observed proportions

Figure 1: Melon organogenesis. Scatterplot

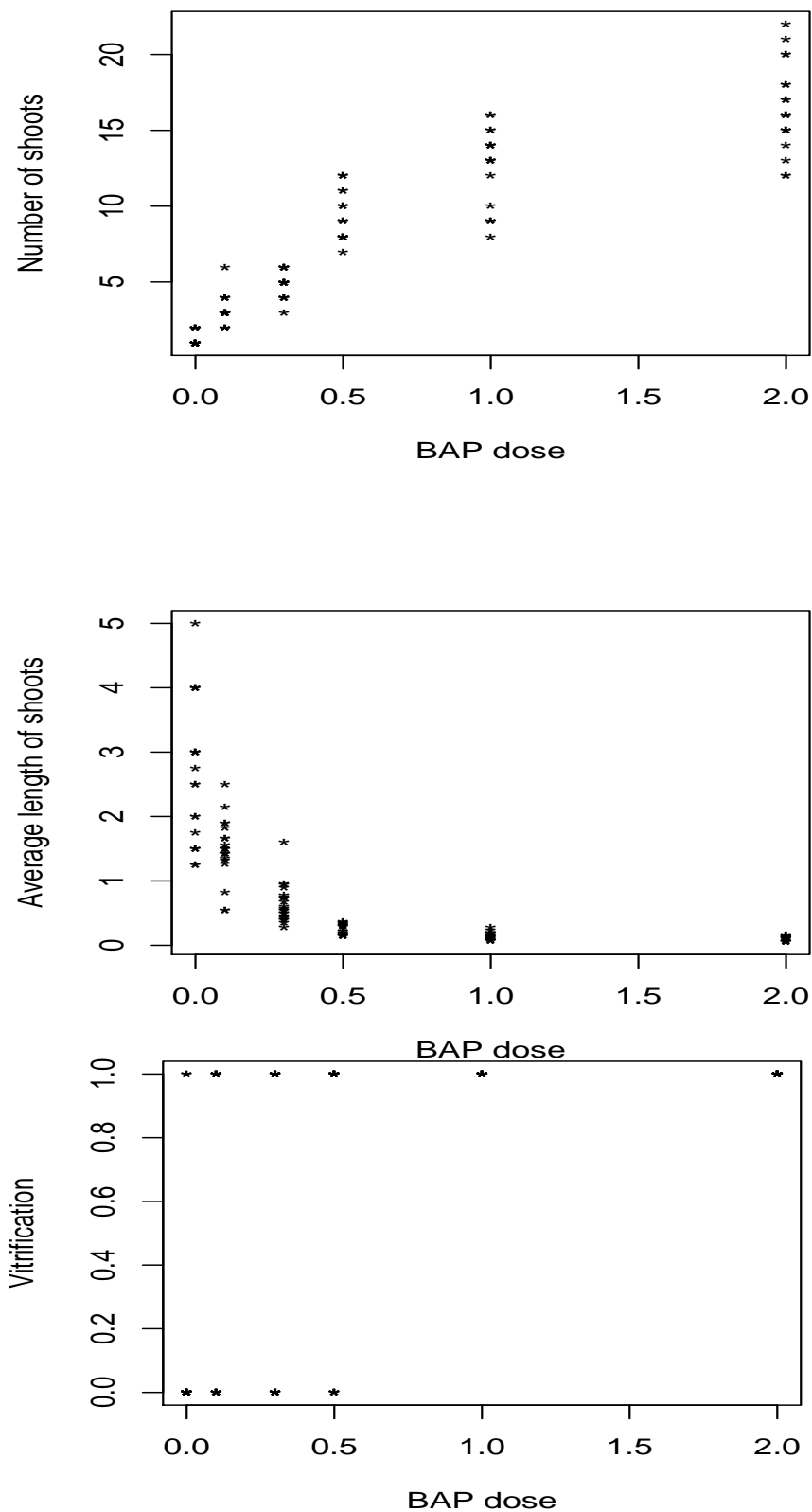


Figure 2: Carnation meristem culture. Scatterplots

Rotenon toxicity

Dose (d_i)	m_i	y_i
0.0	49	0
2.6	50	6
3.8	48	16
5.1	46	24
7.7	49	42
10.2	50	44

- Response variable: Y_i – number of dead insects out of m_i insects (Martin, 1942).
- Distribution: Binomial.
- Systematic component: regression model, completely randomized experiment.
- Aim: Lethal doses.

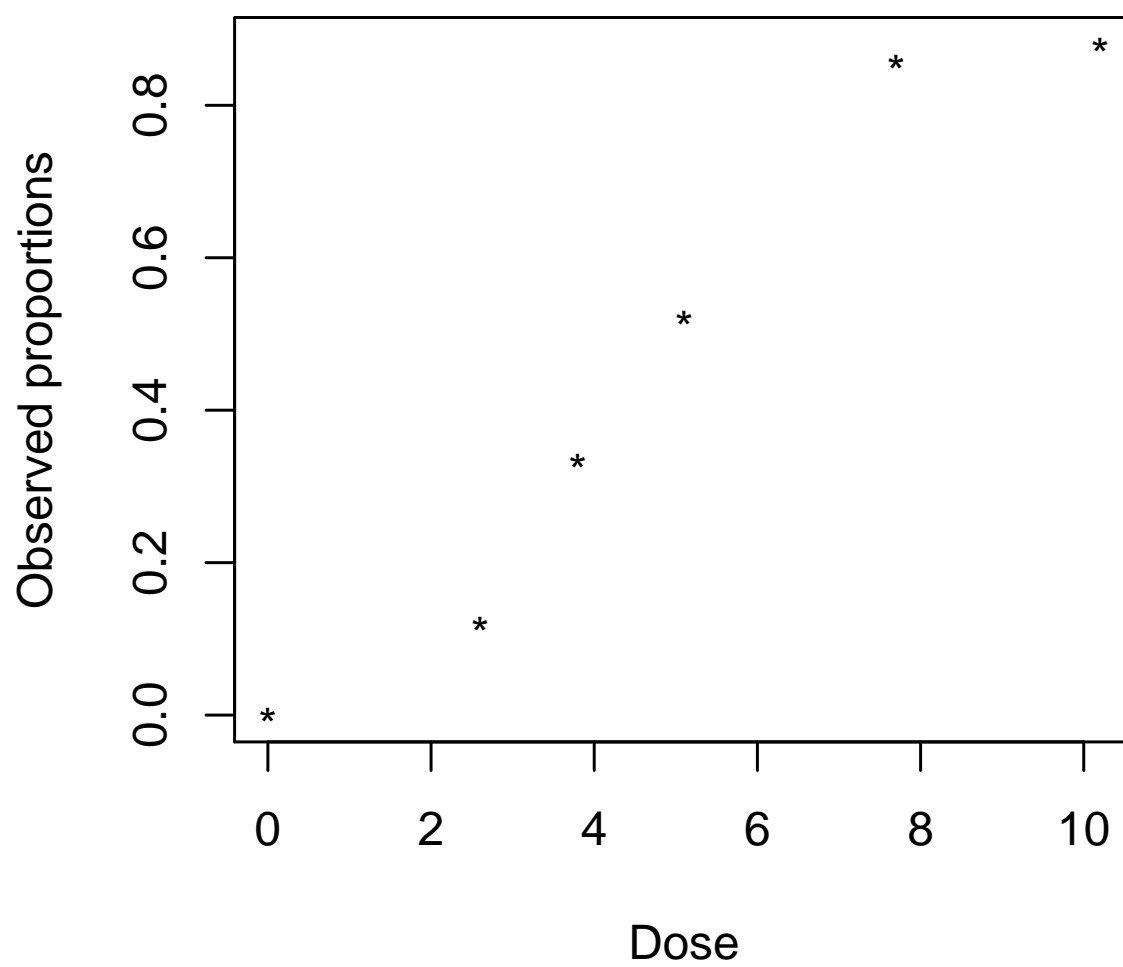


Figure 3: Rotenon - Scatterplot

Germination of Orobanche seed

<i>O. aegyptiaca</i> 75		<i>O. aegyptiaca</i> 73	
Bean	Cucumber	Bean	Cucumber
10/39	5/6	8/16	3/12
23/62	53/74	10/30	22/41
23/81	55/72	8/28	15/30
26/51	32/51	23/45	32/51
17/39	46/79	0/4	3/7
10/13			

Considerations

- Response variable: Y_i – number of germinated seeds out of m_i seeds (Crowder, 1978).
- Distribution: Binomial.
- Systematic component: factorial 2×2 (2 species, 2 extracts), completely randomized experiment.
- Aim: to see how germination is affected by species and extracts.
- Problem: overdispersion.

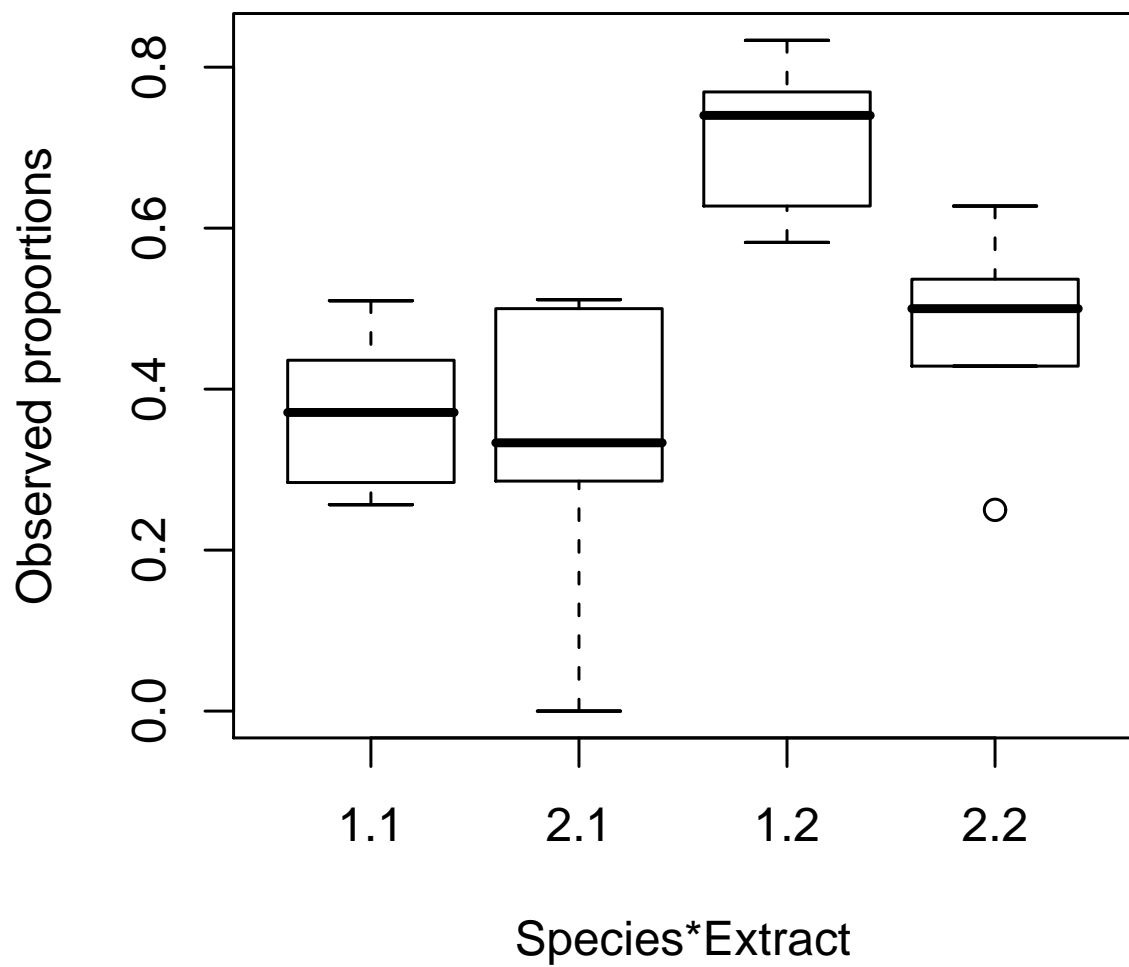


Figure 4: Orobanche - Boxplot

Apple tissue culture

- 4x2 factorial micropropagation experiment of the apple variety Trajan – a 'columnar' variety.
- Shoot tips of length 1.0-1.5 cm were placed in jars on a standard culture medium.
- 4 concentrations of cytokinin BAP added

High concentrations of BAP often inhibit root formation during micropropagation of apples, but maybe not for 'columnar' varieties.

- Two growth cabinets, one with 8 hour photoperiod, the other with 16 hour.

Jars placed at random in one of the two cabinets

- Response variable: number of roots after 4 weeks culture at 22°C.

BAP (μ M)	Photoperiod							
	8				16			
	2.2	4.4	8.8	17.6	2.2	4.4	8.8	17.6
No. of roots								
0	0	0	0	2	15	16	12	19
1	3	0	0	0	0	2	3	2
2	2	3	1	0	2	1	2	2
3	3	0	2	2	2	1	1	4
4	6	1	4	2	1	2	2	3
5	3	0	4	5	2	1	2	1
6	2	3	4	5	1	2	3	4
7	2	7	4	4	0	0	1	3
8	3	3	7	8	1	1	0	0
9	1	5	5	3	3	0	2	2
10	2	3	4	4	1	3	0	0
11	1	4	1	4	1	0	1	0
12	0	0	2	0	1	1	1	0
>12	13,17	13	14,14	14				
No. of shoots	30	30	40	40	30	30	30	40
Mean	5.8	7.8	7.5	7.2	3.3	2.7	3.1	2.5
Variance	14.1	7.6	8.5	8.8	16.6	14.8	13.5	8.5
Overdispersion index	1.42	-0.03	0.13	0.22	4.06	4.40	3.31	2.47

Considerations about the data

- Many zeros for 16 hour photoperiod
- Overdispersion for 16 hour photoperiod
Is this caused by excess zeros?
- Not much overdispersion for the 8 hour photoperiod.
mean \approx variance for concentrations 1, 2 and 4 of BAP.
- For the 8 hour photoperiod the lowest concentration has smallest mean and largest variance
- For the 16 hour photoperiod the conclusion is not so clear cut.

History

The developments leading to the general overview of statistical modelling, known as generalized linear models, extend over more than a century. This history can be traced very briefly as follows (McCullagh & Nelder, 1989, Lindsey, 1997):

- multiple linear regression – a normal distribution with the identity link, $\mu_i = \beta' \mathbf{x}_i$ (Legendre, Gauss, early XIX-th century);
- analysis of variance (ANOVA) designed experiments – a normal distribution with the identity link, $\mu_i = \beta' \mathbf{x}_i$ (Fisher, 1920 to 1935);
- likelihood function – a general approach to inference about any statistical model (Fisher, 1922);
- dilution assays – a binomial distribution with the complementary log-log link, $\log[-\log(1 - \mu_i/m_i)] = \beta' \mathbf{x}_i$ (Fisher, 1922);
- exponential family – a class of distributions

with sufficient statistics for the parameters (Fisher, 1934);

- probit analysis – a binomial distribution with the probit link, $\Phi^{-1}(\mu_i/m_i) = \beta' \mathbf{x}_i$ (Bliss, 1935);
- logit for proportions – a binomial distribution with the logit link, $\log \frac{\mu_i}{m_i - \mu_i} = \beta' \mathbf{x}_i$ (Berkson, 1944, Dyke & Patterson, 1952);
- item analysis – a Bernoulli distribution with the logit link, $\log \frac{\mu_i}{1 - \mu_i} = \beta' \mathbf{x}_i$ (Rasch, 1960);
- log linear models for counts – a Poisson distribution with the log link, $\log \mu_i = \beta' \mathbf{x}_i$ (Birch, 1963);
- regression models for survival data - – an exponential distribution with the reciprocal or the log link, $\frac{1}{\mu_i} = \beta' \mathbf{x}_i$ or $\log \mu_i = \beta' \mathbf{x}_i$ (Feigl & Zelen, 1965, Zippin & Armitage, 1966, Gasser, 1967);
- inverse polynomials – a gamma distribution with the reciprocal link, $\frac{1}{\mu_i} = \beta' \mathbf{x}_i$ (Nelder, 1966).

Generalized Linear Models (glms)

Unifying framework for much statistical modelling.

First introduced by Nelder & Wedderburn (1972) as an extension to the standard normal theory linear model.

- single response variable Y
- explanatory variables x_1, x_2, \dots, x_p ,
($x_1 \equiv 1$)
- random sample: n observations (y_i, \mathbf{x}_i) ,
where $\mathbf{x}_i = (x_{1i}, x_{2i}, \dots, x_{pi})^T$

For more details see, for example:

- McCullagh & Nelder (1989) – theory, applications
- Dobson (2002) – a simple introduction.
- Aitkin *et al* (2009) – practical application of glms using R

Definition of glm

Three components of a generalized linear model are:

- independent random variables Y_i , $i = 1, \dots, n$, from a linear exponential family distribution with means μ_i and constant scale parameter ϕ ,

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

where $\mu = \mathbf{E}[Y] = b'(\theta)$ and $\text{Var}(Y) = \phi b''(\theta)$.

- a linear predictor vector $\boldsymbol{\eta}$ given by

$$\boldsymbol{\eta} = X\boldsymbol{\beta}$$

where $\boldsymbol{\beta}$ is a vector of p unknown parameters and $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]^T$ is the $n \times p$ design matrix;

- a link function $g(\cdot)$ relating the mean to the linear predictor, i.e.

$$g(\mu_i) = \eta_i = \mathbf{x}_i^T \boldsymbol{\beta}$$

Table 1: Identifiers for exponential family distributions

Distribution	$a(\phi)$	θ	$b(\theta)$	$c(y; \phi)$	$\mu(\theta)$	$V(\mu)$
$N(\mu, \sigma^2)$	σ^2	μ	$\frac{\theta^2}{2}$	$-\frac{1}{2} \left[\frac{y^2}{\sigma^2} + \log(2\pi\sigma^2) \right]$	θ	1
$P(\mu)$	1	$\log \mu$	e^θ	$-\log y!$	e^θ	μ
$B(m, \pi)$	1	$\log \left(\frac{\pi}{1-\pi} \right)$	$m \log(1 + e^\theta)$	$\log \binom{m}{my}$	$\frac{e^\theta}{1 + e^\theta}$	$\frac{1}{m} \mu(m - \mu)$
$NB(k)$	1	$\log \left(\frac{\mu}{\mu + k} \right)$	$-k \log(1 - e^\theta)$	$\log \left[\frac{\Gamma(k + y)}{\Gamma(k) y!} \right]$	$k \frac{e^\theta}{1 - e^\theta}$	$\mu \left(\frac{\mu}{k} + 1 \right)$
$G(\mu, \nu)$	ν^{-1}	$-\frac{1}{\mu}$	$-\log(-\theta)$	$\nu \log(\nu y) - \log y - \log \Gamma(\nu)$	$-\frac{1}{\theta}$	μ^2
$IG(\mu, \sigma^2)$	σ^2	$-\frac{1}{2\mu^2}$	$-\frac{1}{2}(-2\theta)$	$-\frac{1}{2} \left[\log(2\pi\sigma^2 y^3) + \frac{1}{\sigma^2 y} \right]$	$(-2\theta)^{-\frac{1}{2}}$	μ^3

Canonical link functions for some distributions

Distribution	Canonical link functions
Normal	Identity: $\eta = \mu$
Poisson	Logarithmic: $\eta = \log(\mu)$
Binomial	Logistic: $\eta = \log\left(\frac{\pi}{1-\pi}\right) = \log\left(\frac{p}{m-p}\right)$
Gamma	Reciprocal: $\eta = \frac{1}{\mu}$
Inverse Gaussian	Reciprocal squared: $\eta = \frac{1}{\mu^2}$

Normal Models

Continuous response variable – Y
Normal distribution, constant variance

$$Y_i \sim N(\mu_i, \sigma^2), \quad i = 1, \dots, n$$
$$\mu_i = \beta_0 + \beta_1 x_{1i} + \dots + \beta_p x_{pi} = \boldsymbol{\beta}^T \mathbf{x}_i$$

- Regression models
continuous explanatory variables
– fitting, testing, model checking
- Analysis of variance
categorical explanatory variables
– *ANOVA* - balanced designs
– *regression* - general unbalanced designs
- Analysis of covariance
mixture of continuous and categorical
explanatory variables

Binomial regression models

Y_i counts of successes out of samples of size m_i ,
 $i = 1, \dots, n$.

Writing

$$\mathbf{E}[Y_i] = \mu_i = m_i \pi_i,$$

a glm models the expected proportions π_i in terms of explanatory variables \mathbf{x}_i

$$g(\pi_i) = \boldsymbol{\beta}' \mathbf{x}_i,$$

For $Y_i \sim \text{Bin}(m_i, \pi_i)$ the variance function is

$$\text{Var}(Y_i) = m_i \pi_i (1 - \pi_i).$$

the canonical link function is the logit

$$g(\mu_i) = \log \left(\frac{\mu_i}{m_i - \mu_i} \right) = \log \left(\frac{\pi_i}{1 - \pi_i} \right) = \eta_i$$

Other common choices are

- probit $g(\mu_i) = \Phi^{-1}(\mu_i/m_i) = \Phi^{-1}(\pi_i)$
- complementary log-log (CLL) link

$$g(\mu_i) = \log\{-\log(1 - \pi_i)\}.$$

Poisson regression models

If Y_i , $i = 1, \dots, n$, are counts with means μ_i , the standard Poisson model assumes that $Y_i \sim \text{Pois}(\mu_i)$ with variance function

$$\text{Var}(Y_i) = \mu_i.$$

The canonical link function is the log

$$g(\mu_i) = \log(\mu_i) = \eta_i,$$

For different observation periods/areas/volumes:

$$Y_i \sim \text{Pois}(t_i \lambda_i)$$

Taking a log-linear model for the rates,

$$\log(\lambda_i) = \mathbf{x}_i^T \boldsymbol{\beta}$$

results in the following log-linear model for the Poisson means

$$\log(\mu_i) = \log(t_i \lambda_i) = \log(t_i) + \mathbf{x}_i^T \boldsymbol{\beta},$$

where the $\log(t_i)$ is included as a fixed term, or *offset*, in the model.

Estimation and model fitting

- Maximum likelihood estimation.
- Estimation algorithm (Nelder & Wedderburn, 1972)
 - Iteratively weighted least squares (IWLS)

$$X^T W X \boldsymbol{\beta} = X^T W \mathbf{z}$$

where

$X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]^T$ is a design matrix $n \times p$,

$W = \text{diag}\{W_i\}$ – depends of the prior weights, variance function (distribution) and link function

$$W_i = \frac{1}{V(\mu_i)} \left(\frac{d\mu_i}{d\eta_i} \right)^2$$

$\boldsymbol{\beta}$ – parameter vector $p \times 1$

\mathbf{z} – a vector $n \times 1$ (adjusted response variable) – depends on y and link function

$$z_i = \eta_i + (y_i - \mu_i) \frac{d\eta_i}{d\mu_i}$$

Inferential aspects

Measures of discrepancy:

Deviance

$$S = \frac{D}{\phi} = -2[\log L(\hat{\boldsymbol{\mu}}, \mathbf{y}) - \log L(\mathbf{y}, \mathbf{y})]$$

where $L(\hat{\boldsymbol{\mu}}, \mathbf{y})$ e $L(\mathbf{y}, \mathbf{y})$ are the likelihood function values for the current and saturated models

Generalized Pearson X^2

$$X^2 = \sum \frac{(y_i - \hat{\mu}_i)^2}{V(\hat{\mu}_i)}$$

- In general, comparisons involve nested models and deviance differences (Analysis of deviance).
- Many interesting comparisons involve non-nested models
- Use of Akaike Information Criterion (AIC) or Bayes Information Criterion (BIC) for model selection

AIC = $-2 \log L + 2$ (number of fitted parameters)

BIC = $-2 \log L + \log n$ (number of fitted parameters)

- When the dispersion parameter is unknown, it may be estimated by the Pearson Estimator

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

where $\hat{\mu}_i = g^{-1}(\hat{\beta}' \mathbf{x}_i)$ is the i th fitted value.

- Some computer packages estimate ϕ by the deviance estimator $D(\hat{\beta})/(n-p)$; but it cannot be recommended because of problems with bias and inconsistency in the case of a non-constant variance function.
- For positive data, the deviance may also be sensitive to rounding errors for small values of y_i .
- The asymptotic variance of $\hat{\beta}$ is estimated by the inverse (Fisher) information matrix, giving

$$\text{Var}(\hat{\beta}) = \mathbb{K} = \phi(\mathbb{X}^T \mathbb{W} \mathbb{X})^{-1},$$

where \mathbb{W} is calculated from $\hat{\beta}$.

- The standard error $\text{se}(\hat{\beta}_j)$ is calculated as the square-root of the j th diagonal element of this matrix, for $j = 1, \dots, p$

- When ϕ is known, a $1 - \alpha$ confidence interval for β_j is defined by the endpoints

$$\hat{\beta}_j \pm \text{se}(\hat{\beta}_j) z_{1-\alpha/2}$$

where $z_{1-\alpha/2}$ is the $1 - \alpha/2$ standard normal quantile.

- For ϕ unknown, we replace ϕ by $\hat{\phi}$ in \mathbb{K} and a $1 - \alpha$ confidence interval for β_j is defined by the endpoints

$$\hat{\beta}_j \pm \text{se}(\hat{\beta}_j) t_{(1-\alpha/2)}(n - p)$$

where $t_{(1-\alpha/2)}(n - p)$ is the $1 - \alpha/2$ quantile of Student's t distribution with $n - p$ degrees of freedom.

Analysis of Deviance – Goodness of fitting and model selection

- Analysis of deviance is the method of parameter inference for generalized linear models based on the deviance, generalizing ideas from ANOVA, and first introduced by Nelder and Wedderburn (1972).
- The situation is similar to regression analysis, in the sense that model terms must be eliminated sequentially, and the significance of a term may depend on which other terms are in the model.
- The deviance D measures the distance between y and $\hat{\mu}$, given by

$$S = \frac{D(\hat{\beta})}{\phi} = -2[\log L(\hat{\mu}, y) - \log L(y, y)] = 2\phi^{-1} \sum_{i=1}^n w_i [y_i(\tilde{\theta}_i - \hat{\theta}_i)]$$

where $L(\hat{\mu}, y)$ and $L(y, y)$ are the likelihood function values for the current and saturated models, $\tilde{\theta}_i = \theta(y_i)$, $\hat{\theta}_i = \theta(\hat{\mu}_i)$ and $D(\hat{\beta}) = \sum_{i=1}^n w_i d(y_i; \hat{\mu}_i)$.

Deviance for some models

Model	Deviance
Normal	$D_p = \sum_{i=1}^n (y_i - \hat{\mu}_i)^2$
Binomial	$D_p = 2 \sum_{i=1}^n \left[y_i \log \left(\frac{y_i}{\hat{\mu}_i} \right) + (n_i - y_i) \log \left(\frac{n_i - y_i}{\hat{\mu}_i} \right) \right]$
Poisson	$D_p = 2 \sum_{i=1}^n \left[y_i \log \left(\frac{y_i}{\hat{\mu}_i} \right) + (\hat{\mu}_i - y_i) \right]$
Negative Binomial	$D_p = 2 \sum_{i=1}^n \left[y_i \log \left(\frac{y_i}{\hat{\mu}_i} \right) + (y_i + k) \log \left(\frac{y_i + k}{\hat{\mu}_i} \right) \right]$
Gamma	$D_p = 2 \sum_{i=1}^n \left[\log \left(\frac{\hat{\mu}_i}{y_i} \right) + \frac{y_i - \hat{\mu}_i}{\hat{\mu}_i} \right]$
Inverse Gaussian	$D_p = \sum_{i=1}^n \frac{(y_i - \hat{\mu}_i)^2}{y_i \hat{\mu}_i^2}$

- We consider separately the cases where ϕ is known and unknown, but first we introduce some notation.
- Let M_1 denote a model with p parameters, and let $D_1 = D(\hat{\beta})$ denote the minimized deviance under M_1
- Let M_2 denote a sub-model of M_1 with $q < p$ parameters, and let D_2 denote the corresponding minimized deviance, where $D_2 \geq D_1$

Known dispersion ϕ parameter

- Mainly relevant for discrete data, for which, in general, $\phi = 1$.
- The deviance D_1 is a measure of goodness-of-fit of the model M_1 ; and is also known as the G^2 statistic in discrete data analysis.
- A more traditional goodness-of-fit statistic is Pearson's X^2 statistic

$$X^2 = \sum \frac{w_i (y_i - \hat{\mu}_i)^2}{V(\hat{\mu}_i)}$$

- Asymptotically, for large w the statistics D_1 and X^2 are equivalent and distributed as $\chi^2(n - p)$ under M_1 .
- Various numerical and analytical investigations have shown that the limiting χ^2 distribution is approached faster for the X^2 statistic than for D_1 , at least for discrete data.

- A formal level α goodness-of-fit test for M_1 is obtained by rejecting M_1 if
$$X^2 > \chi^2_{(1-\alpha)}(n - p)$$
- This test may be interpreted as a test for overdispersion.
- The fit of a model is a complex question, cannot be summarized in a single number – supplement with an inspection of residuals.

- To test the sub-model M_2 with $q < p$ we use the log likelihood ratio statistic

$$D_2 - D_1 \sim \chi^2(p - q)$$

- M_2 is rejected at level α if $D_2 - D_1 > \chi^2_{(1-\alpha)}(p - q)$
- In the case where $\phi \neq 1$ we use the scaled deviance D/ϕ instead of D ; and the scaled Pearson statistic X^2/ϕ instead of X^2 and so on.

Unknown dispersion ϕ parameter

- The dispersion parameter is usually unknown for continuous data
- In the discrete case we may prefer to work with unknown dispersion parameter, if evidence of overdispersion has been found in the data.
- There is no formal goodness-of-fit test available based on X^2 – the fit of the model M_1 to the data must be checked by residual analysis.
- X^2 is used to estimate the dispersion parameter

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

where $\hat{\mu}_i = g^{-1}(\hat{\beta}' \mathbf{x}_i)$ is the i th fitted value.

- To test the sub-model M_2 with $q < p$ parameters inference may be based on

F -statistic,

$$F = \frac{(D_2 - D_1)/(p - q)}{\hat{\phi}} \sim F(p - q, n - p)$$

- We reject M_2 at level α if $F > F_{1-\alpha}(p - q, n - p)$

Table 2: Deviance Table – An example.

Model	DF	Deviance	Deviance Diff.	DF Diff.	Meaning
Null	$rab - 1$	D_1			
			$D_1 - D_A$	$a - 1$	A ignoring
A	$a(rb - 1)$	D_A			
			$D_A - D_{A+B}$	$b - 1$	B including
A+B	$a(rb - 1) - (b - 1)$	D_{A+B}			
			$D_{A+B} - D_{A*B}$	$(a - 1)(b - 1)$	Interaccion included A and B
A+B+A.B	$ab(r - 1)$	D_{A*B}			
			D_{A*B}	$ab(r - 1)$	Residual
Saturated	0	0			

Residual analysis

- **Pearson residual**

$$r_{Pi} = \frac{y_i - \hat{\mu}_i}{\sqrt{V(\hat{\mu}_i)}}$$

reflect the skewness of the underlying distribution.

- **Deviance residual**

$$r_{Di} = \text{sign}(y_i - \hat{\mu}_i) \sqrt{d(y_i; \hat{\mu}_i)}$$

which is much closer to being normal than the Pearson residual, but has a bias (Jorgensen, 2011).

- **Modified deviance residual** (Jorgensen, 1997)

$$r_{Di}^* = r_{Di} + \frac{\phi}{r_{Di}} \log \frac{r_{Wi}}{r_{Di}}$$

where r_{Wi} is the Wald residual defined by

$$r_{Wi} = [g_0(y_i) - g_0(\mu_i)] \sqrt{V(y_i)}$$

where g_0 is the canonical link.

- All those residuals have approximately mean zero and variance $\phi(1 - h_i)$, where h_i is the i th diagonal element of the matrix $\mathbb{H} = \mathbb{W}^{1/2}\mathbb{X}(\mathbb{X}^T\mathbb{W}\mathbb{X})^{-1}\mathbb{X}^T\mathbb{W}^{1/2}$.
- Use standardized residuals such as $r_{Di}^*(1 - h_i)^{1/2}$, which are nearly normal with variance ϕ
- Plot residuals against the fitted values – to check the the proposed variance function
- Normal Q-Q plot (or normal Q-Q plot with simulated envelopes) for the residuals – to check the correctness of the distributional assumption

R commands for GLM

```
glm(resp ~ linear predictor + offset(of), weights = w,  
family=familyname(link = "linkname" ))
```

The *resp* is the response variable y . For a binomial regression model it is necessary to create:

```
resp<-cbind(y,n-y)
```

The possible families ("canonical link") are:

```
binomial(link = "logit")  
gaussian(link = "identity")  
Gamma(link = "inverse")  
inverse.gaussian(link = "1/mu^2")  
poisson(link = "log")  
quasi(link = "identity", variance = "constant")  
quasibinomial(link = "logit")  
quasipoisson(link = "log")
```

The default family is the gaussian family and default links are the canonical links (don't need to be declared). Other possible links are "probit", "cloglog", "cauchit", "sqrt", etc. To see more, type

```
? glm
```


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