Generalized Linear Models

- The family of *generalized linear models* (GLM) encompasses several regression models, which are all based on exponential distribution family.
- These models are specified by implementing a linear predictor $\eta_i = \mathbf{x}_i^T \cdot \boldsymbol{\beta}$ in either metric or categorical variables, or a combination thereof, that is ***linked*** to the expected value.
- GLM's flexibility, while using one unified estimation procedure, makes it very appealing model class.
- Several extensions are available that allow relaxing some underlying assumptions of GLM.

The Exponential Family (not test relevant)

- The general structure of a distribution function from the exponential family is

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

with θ being a ***location parameter***, such as the expected value $E(y) = \theta$, and ϕ being a scale parameter.

- Many distribution functions, such as the ***normal***, the ***exponential***, the ***binomial***, the ***Gamma*** and the ***Poisson*** distribution are members of the exponential family and thus can be estimate with the GLM approach.

The linear predictor η_i and the expected value θ_i are connected through a link function $link(\theta_i) = \eta_i$. For example, for binary logistic model the link function becomes the logit $\log\left(\frac{\pi_i}{1-\pi_i}\right) = \eta_i$ with $\theta_i \equiv \pi_i$.

Table 5.2 Default (canonical) link, response range, and conditional variance function for generalized linear model families; ϕ is the dispersion parameter, η_i is the linear predictor, and μ_i is the expectation of y_i (the response). In the binomial family, n_i is the number of trials.

Family	*Default Link*	*Range of* y_i	$V(y_i\|\eta_i)$
`gaussian`	`identity`	$(-\infty, +\infty)$	ϕ
`binomial`	`logit`	$\frac{0,1,\ldots,n_i}{n_i}$	$\mu_i(1-\mu_i)$
`poisson`	`log`	$0, 1, 2, \ldots$	μ_i
`Gamma`	`inverse`	$(0, \infty)$	$\phi\mu_i^2$
`inverse.gaussian`	`1/mu^2`	$(0, \infty)$	$\phi\mu_i^3$

- For the Poisson distribution, which is used as main example throughout this lecture, we get the specification as a member of the exponential distribution as

$$\boxed{f(y;\mu) = \frac{\exp(-\mu)\cdot\mu^y}{y!}} = \exp\left[y\cdot\ln\mu - \mu - \ln(y!)\right]$$

Poisson distribution

mu is the intensity

with $\theta = \ln\mu$, $b(\theta) = \mu \Leftrightarrow b(\theta) = \exp(\theta)$, $c(y,\phi) = -\ln(y!)$ and $a(\phi) = 1$. Thus, the location parameter is μ and the scale parameter is constant $\phi = 1$.

- A generic maximum likelihood estimation procedure exists for all members of the exponential family. One possible estimation procedure is the ***iteratively reweighted regression*** algorithm.

Likelihood and Iteratively Reweighted Regression for the Poisson Distribution (not test relevant)

- Let $\mu_i = \exp(\mathbf{x}_i^T \cdot \boldsymbol{\beta})$ with $E(y_i) = \mu_i$ and $Var(y_i) = \mu_i$ according to the Poisson distribution. That means the variance of the Poisson distribution is ***restricted*** to be equal to its expectation: $E(Y_i) = Var(Y_i) = \mu_i$.
- By making use of the exponential family specification, the log-likelihood function becomes

$$\ln L(\boldsymbol{\beta};\mathbf{y}) = \ln\left(\prod_{i=1}^{n} \exp\left[y_i \cdot \ln\mu_i - \mu_i - \ln(y_i!)\right]\right)$$

$$= \sum_{i=1}^{n}\left[y_i \cdot \underbrace{\left(\mathbf{x}_i^T \cdot \boldsymbol{\beta}\right)}_{=\ln\exp(\mathbf{x}_i^T \cdot \boldsymbol{\beta})} - \exp\left(\mathbf{x}_i^T \cdot \boldsymbol{\beta}\right) - \ln(y_i!)\right]$$

- The first derivatives are

$$\frac{\partial \ln L(\boldsymbol{\beta};\mathbf{y})}{\partial \boldsymbol{\beta}} = \sum_{i=1}^{n}\left[y_i \cdot \mathbf{x}_i - \exp(\mathbf{x}_i^T \cdot \boldsymbol{\beta}) \cdot \mathbf{x}_i^T\right]$$

- Evaluate the derivatives at zero gets a system of nonlinear equations

$$\sum_{i=1}^{n}\left[y_i-\underbrace{\exp(\mathbf{x}_i^T\cdot\boldsymbol{\beta})}_{\hat{\mu}_i}\right]\cdot\mathbf{x}_i^T \Leftrightarrow \mathbf{X}^T\cdot\left[\mathbf{y}-\underbrace{\exp\left(\mathbf{X}\cdot\boldsymbol{\beta}\right)}_{\hat{\boldsymbol{\mu}}}\right]$$

Similar constraints were observed for the OLS model and the logistic regression model, which lead to unbiased predictions.

Note: This constraint does not hold, however, to the negative binomial model. Thus its predictions are biased.

- Alternatively, the maximization problem can be specified as weighted regression where we minimize the weighted sum of squares S_{χ^2} with

$$S_{\chi^2}=\sum_{i=1}^{n}\frac{\left(y_i-\mu_i\right)^2}{\mu_i}$$

The weight here is the inverse of the expected variances: $1/\mu_i$

- The first derivative gives

$$\begin{aligned}\frac{\partial S_{\chi^2}}{\partial\boldsymbol{\beta}}&=2\cdot\sum_{i=1}^{n}\frac{\left[y_i-\exp(\mathbf{x}_i^T\cdot\boldsymbol{\beta})\right]\cdot\exp(\mathbf{x}_i^T\cdot\boldsymbol{\beta})\cdot\mathbf{x}_i^T}{\exp(\mathbf{x}_i^T\cdot\boldsymbol{\beta})}\\&=2\cdot\sum_{i=1}^{n}\left[y_i-\exp(\mathbf{x}_i^T\cdot\boldsymbol{\beta})\right]\cdot\mathbf{x}_i^T\end{aligned}$$

- This is equivalent to the maximum likelihood estimator.

- Note: use has been made of the quotient rule of differentiation:
  $$\frac{\partial}{\partial x}\frac{f(x)}{g(x)} = \frac{1}{g(x)}\frac{\partial f(x)}{\partial x} - \frac{f(x)}{g^2(x)}\frac{\partial g(x)}{\partial x}.$$
- See Fox & Weisberg section 5.12 for the specification of the iteratively reweighted least squares algorithm as a first order Taylor Series expansion

Specification Decisions for GLM

- First, one needs to decide how the dependent (response) variable y_i is distributed. Its distribution should come from the exponential family. This ***defines the likelihood function*** to be used.
  - For example:

    [a] count data $y \in \{0,1,2,\ldots\}$ without an upper ceiling follow a ***Poisson*** distribution

    [b] binary $y \in \{0,1\}$ realizations follow a ***binary*** distribution,

    [c] whereas counts within a ***fixed range*** $y \in \{0,1,\ldots,n\}$ follow a ***binomial*** distribution.
  - For most members of the exponential family, their ***scale depends*** on the location parameter and ***cannot*** vary freely.

    This is a fairly restrictive property of these distributions, which however can be relaxed through a ***quasi-likelihood*** specification by allowing for ***over-*** or ***underdispersion*** of the variances.

    However, for quasi-likelihood model the likelihood becomes undefined.

- Second, one needs to decide within limits how the expectations θ_i of the individual observations y_i are ***linked*** to their linear predictor η_i.
  - The limits of the link need to ensure that the expectation remains within the feasible range of the underlying distribution. E.g.: $\pi \in [0,1]$ for the *logistic* and *probit* regression and $\mu > 0$ for Poisson regression.
  - The literature usually expresses the linear predictor by $\eta_i = \mathbf{x}_i^T \cdot \boldsymbol{\beta}$ and connects the expectation $E[y_i] = \theta_i$ to η_i with a *link function*

$$link\left(\underbrace{E[y_i]}_{=\theta_i}\right) = \eta_i \text{ with } \eta_i = \mathbf{x}_i^T \cdot \boldsymbol{\beta}$$

For the Poisson model it is $\log(\mu_i) = \eta_i = \mathbf{x}_i^T \cdot \boldsymbol{\beta}$ and for logistic regression it is $\text{logit}(\pi_i) = \log\left(\frac{\pi_i}{1-\pi_i}\right) = \eta_i$.

Table 5.3 Family generators and link functions for `glm`: S, available in S-PLUS; R, available in R. In each case, the default link is shown in boldface.

	link							
family	identity	inverse	log	logit	probit	cloglog	sqrt	1/mu^2
gaussian	$\boxed{\textbf{S,R}}$	R	R					
binomial			R	**S,R**	S,R	S,R		
poisson	S,R		**S,R**				S,R	
Gamma	S,R	**S,R**	S,R					
inverse.gaussian	R	R	R					**R**
quasi	**S,R**	S,R	S,R	S,R	S,R	S,R	S,R	S,R
quasibinomial				**R**	R	R		
quasipoisson	R		**R**				R	

- The ***inverse link*** function is an expression in terms of the expectation $\boxed{\mu_i = E[y_i] = link^{-1}(\eta_i)\,.}$
  - For logistic regression it becomes the inverse logit function and for Poisson regression it is the exponential function.
- At this point one may wonder how the link function differs from applying a transformation on the dependent variable (e.g., the Box-Cox transformation)? The quick answer is that the link function actually transforms the ***expected*** value $link(E[y_i])$ of the dependent variable and not on the ***dependent*** variable y_i itself.

Extension 1: Quasi-Likelihood and Over- and Under-dispersion

- The scale parameter ϕ in logistic and Poisson regression is equal to 1 due to the properties of the underlying distributions.
- However, the estimated variance of the response variable may not satisfy the constraint $Var(y_i) = E(y_i)$ for the Poisson model and $Var(y_i) = \frac{\pi_i \cdot (1-\pi_i)}{n_i}$ with $E(y_i) = \pi_i$ for the binomial model.
- Potential reasons for observing excess dispersion are:
  - For the logistic model: Due to ***missing information*** the true predicted expectation may vary among grouped observations, even though they are identically in their observed exogenous variables. This is a classic case of ***model misspecification***.
  - For Poisson regression: GLM assumes independence among the observations. It may however happen that the aggregated counts over time and/or space in one observation y_i are ***correlated*** with other counts.

    For instance, the number of persons migrating is most likely correlated because we count family members as if they move independently whereas they move jointly as a "clan".
  - An ***incorrect assumption*** about the distributional model.
  - The choice of the link function is incorrect.
  - There are outliers in the data.

- Under- and over-dispersion may lead to poorly fitting models.
- The estimated regression coefficients remain ***unbiased***, however, their ***standard error*** comes incorrect, which prohibits us from assessing their statistical significance correctly (recall OLS estimates under heteroscedasticity or autocorrelation).
- ***Quasi-Poisson*** and ***Quasi-Binomial*** GLM regression adjusts the standard errors properly and allows to estimate the dispersion parameter ϕ.
- A dispersion parameter $\boxed{\phi \gg 1}$ indicates the presences of ***over***-dispersion whereas $\phi \ll 1$ indicates ***under***-dispersion.

  The dispersion parameter is the ratio of the empirical χ^2-value of the model's squared Pearson residuals and its expectation $E\left(\chi^2\right) = df$, which is the degrees of freedom of the model.

Extension 2: Negative Binomial Model

- Another approach of dealing with over-dispersion in a Poisson model is to switch to a ***negative binomial*** distribution. The function **`glm.nb`** in the MASS library allows estimating these models.

  Unfortunately, the negative binomial model may lead to ***biased*** predicted values.
- See Fox & Weisberg (2nd edition) pp 278-281 for a discussion and examples.

Extension 3: The Offset Term

- Sometimes an *a priori* baseline expectation $E(y_i \mid H_0)$ is available for the response variable and we are interested in how the exogenous variables influence the ***variation*** of the individual expectations μ_i around their baseline expectations.
    - For example: In migration studies the observed flow m_{ij} between two regions i and j is modeled by a set of origin and destination characteristics and their intervening distance. One can expect that the current migration flow m_{ij}^t does not differ much from the flow of the previous period m_{ij}^{t-1}. Therefore, m_{ij}^{t-1} can be the baseline expectation.
- For a Poisson regression model one could think of defining a new dependent variable as $\mu_i / E(y_i \mid H_0)$ and start modeling

$$\log\left(\mu_i / E[y_i \mid H_0]\right) = \eta_i \Leftrightarrow \log(\mu_i) - \log(E[y_i \mid H_0]) = \eta_i .$$

- However, the distribution of $\log(\mu_i) - \log(E[y_i \mid H_0])$ is usually not known or does not belong to the exponential family.
- One can combine the baseline expectation with a ***fixed regression coefficient*** equal to one with the linear predictor η_i because both are given exogenously.

  This leads to the ***offset*** specification of the Poisson regression model

$$\boxed{\log(\mu_i) = \eta_i + \underbrace{1}_{fixed} \cdot \log(E[y_i \mid H_0])}$$

- The term $\log(E[y_i \mid H_0])$ is called the offset. It needs to be given in its proper *log*-format for the Poisson regression model.

Special GLM Models

The Multinomial Logistic Model

- See Fox & Weisberg (2nd edition) pp 259-268

The Proportional Odds model for Ordered Response Variables

- See Fox & Weisberg (2nd edition) pp 269-272

The Log-Linear Model for Multidimensional Contingency Tables

- See Fox & Weisberg (2nd edition) pp 250-256 for examples and discussion.
- Discuss the meaning of interaction terms and their implications of on the predicted values in partial contingency tables (or the marginal counts).
- Iterative Proportional Fit algorithm can be used to generate predicted tables that satisfy the constraints of [a] externally give ***marginal counts*** and [b] of having a given *a priori* ***interdependence structure*** among the factors. The resulting table will satisfy both constraints.
- See **`IterPropFitWithInitial.r`** for an implementation.

Zero Inflated Poisson Regression

- One needs to distinguish ***random zero*** form ***structural zeros***.

  - Random zero: one could have observed a count other than zero, so an observed zero is just a ***chance realization*** of the underlying random process.
  - Structural zero: It is ***impossible*** to observe a particular cell count on ***logical grounds***. Thus, records associated with cells for which only structural zeros are possible need to be excluded from the analysis.
    They are not members of the underlying population from which a sample has been taken.
- If the data have more random zeros than expected based on the underlying probability model then a zero inflated Poisson regression model can be selected.
- It uses a mixture distribution approach to model the random zeros:
  - the first component distribution models the probability for observing a ***zero count*** and
  - the second component distribution models the probability of observing a ***truncated Poisson distributed count*** ranging from $y \in \{1, 2, \ldots\}$, i.e., a Poisson distribution without zeros.
- See the R function **`zeroinfl`** in the package **`pscl`** for estimation details and *ZeroInflatedPoisson.pdf* for a discussion.
- This model is, for instance, applicable to sparsely populated cross-tabulations. For particular table cells not observations are made due to a small sample size. Here the first component distribution models the likelihood of making an observation for each cell.

Example: Basic Disease Modeling

Logistic Regression:

- Let x_i be and observed disease count (either standardized or unstandardized), which is related to a population at risk N_i.
- Then x_i follows a binomial distribution with $\Pr(X_i = x_i) = \frac{N_i!}{x_i! \cdot (N_i - x_i)!} \cdot \pi_i^{x_i} \cdot (1 - \pi_i)^{(N_i - x_i)}$ instead of a binary distribution.
- To model the observed disease rate $r_i = \frac{x_i}{N_i}$ the **`glm`** function for logistic regression needs to know what the given population at risk is in order to model the variance $\frac{\pi_i \cdot (1-\pi_i)}{N_i}$ of each observation properly. This is achieved with the statement **`glm(r~., weights=N, family=binomial)`** where $\mathbf{r} = (r_1, \ldots, r_n)^T$ and $\mathbf{N} = (N_1, \ldots, N_n)^T$.

Poisson Regression:

- For rare diseases, that is, $\pi_i \cong 0$, the binomial distribution can be approximated by the Poisson distribution.
- To account for the varying population at risk sizes, one focuses on the standardized mortality ratios $SMR_i = \frac{x_i}{e_i}$, where e_i is the expected count based on indirect standardization.
- The Poisson regression internally models the expected value of the observed counts with a log-link function $\log(E(x_i)) \equiv \log(\lambda_i)$

- Since the expected counts e_i are assumed to be deterministic, the expression becomes for the standardized mortality ratios $\log(E(SMR_i)) = \log(E(x_i)) - \log(e_i)$.
- The expression for Poisson regression of observed disease counts adjusted by the expected counts becomes **`glm(x~., offset(log(e)), family=poisson)`** where the log-transformed vector of expected counts $\mathbf{e} = (e_1, \dots, e_n)^T$ is brought in as offset to the right-hand side of the equation.
- Offsets have a ***fixed*** regression coefficient of ***one***.

Example: The Rudimentary Spatial Interaction Model

- Let the expected flow between an origin i to a destination j be specified as

$$E(m_{ij}) = \mu_{ij} = \beta_0 \cdot \frac{p_i^{\beta_1} \cdot p_j^{\beta_2}}{d_{ij}^{\beta_3}}$$

  where m_{ij} is the observed flow between origin i and destination j, p_i is an origin characteristic (such as the origin population) and p_j a destination attribute (such as the destination population) and d_{ij} a measure of separation between i and j.

- The dependent variable m_{ij} is a count ranging from $m_{ij} \in \{0,1,2, \dots, \infty\}$. Therefore, the assumption $m_{ij} \sim Poisson(\mu_{ij} | p_i, p_j, d_{ij})$ is appropriate.
- The link function $\ln(\mu_{ij}) = \eta_{ij}$ allows modeling the observed flows with

$$\eta_{ij} = \ln(\beta_0) + \beta_1 \cdot \ln(p_i) + \beta_2 \cdot \ln\left(p_j\right) - \beta_3 \cdot \ln(d_{ij})$$

by a Poisson regression model.