#### Phd Program in Transportation

#### **Transport Demand Modeling**

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# **Generalized Linear Models**

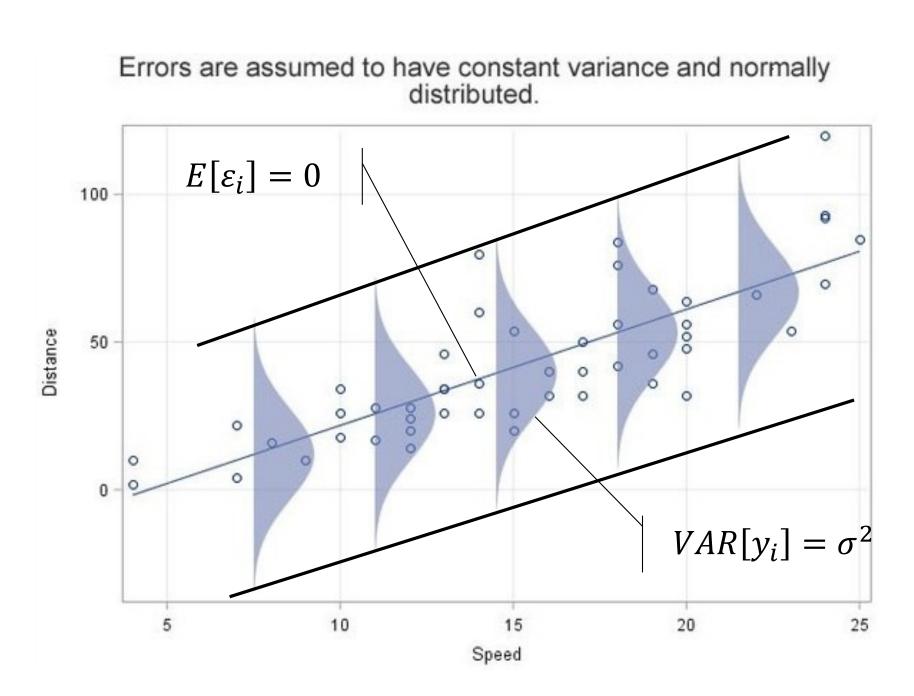
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# Why Generalized Linear Models?

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#### □ Why using GZLM?

- We shall see that these models extend the linear modelling framework to models where:
  - The dependent variable may not be continuous
  - > The effect of independent variables may not be linear
  - > The expected value of the errors terms might not be 0.
- GZLM unify all non linear models, used to explain the situation were the linear normal regression was not able to explain the relation under analysis
- GZLMs are most commonly used to model binary or count data, so we will focus on models for these types of data.





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# When do GZLM come into play?

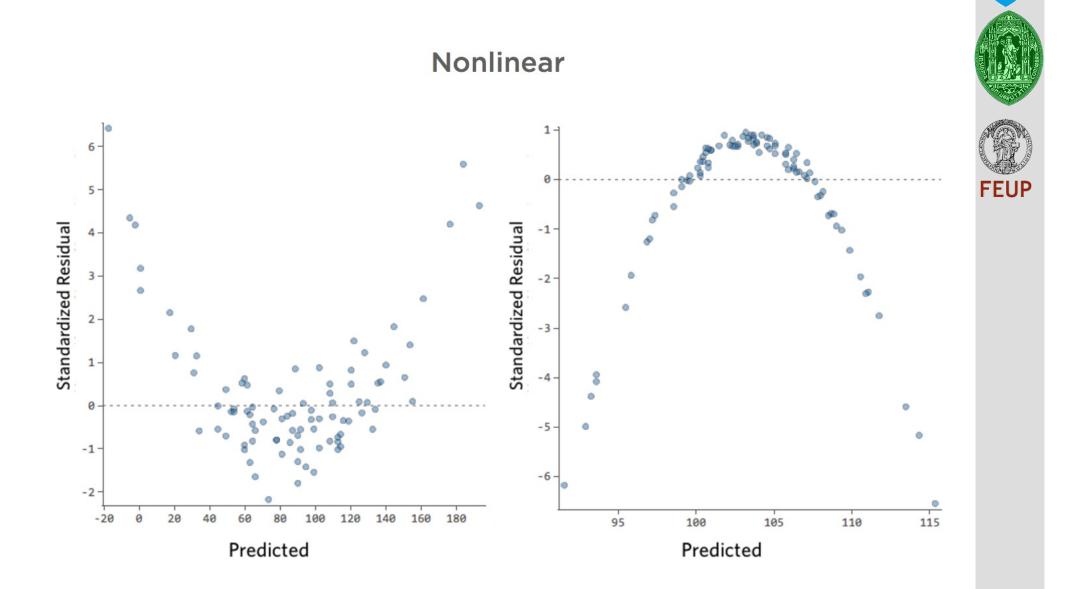
#### **With MLR**:

- >  $Y_i = BX + \varepsilon$ , where X is a vector of predictors and B is a vector of coefficients  $\beta$
- $\succ E[Y_i] = \widehat{B}X$  because  $E[\varepsilon_i] = 0$  and  $VAR[y_i] = \sigma^2$

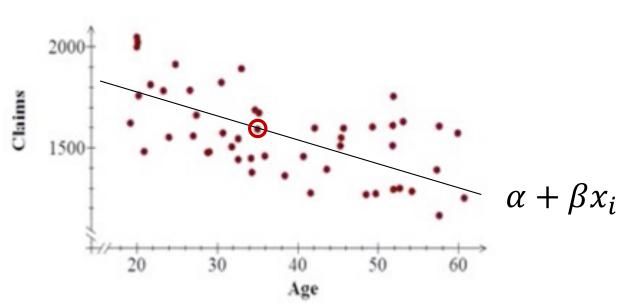
- When such conditions are not met,
  - > When  $E[\varepsilon_i] \neq 0$  or  $VAR[Y_i] \neq \sigma^2$
- $\hfill\square$  you use GZLM where...
  - The variation (probabilistic distribution) in the response variable Yi can be explained in terms of the values of X
  - We want to find some link function g(.), that mediates the response variable (Yi) and the regressors Xi, such that

 $E[g(Y_i)] = \widehat{B}X$ , where g(.) is the link function.





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#### **Recap on linear models and generalizing**

- $\Box$  Distributions of the Y's:
- $Y_i \sim N(\mu_i, \sigma^2)$
- $\Box$  Function of the explanatory variable,  $x_i$ 's:  $\alpha + \beta x_i$
- $\Box$  Connection between explanatory variable and the distribution of  $Y_i$ :

$$\mu_i = E[Y_i] = \alpha + \beta x_i$$

We will now generalize the distribution of the Yi variables according to different distributions, besides the normal distribution FEUP

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n  $var(Y_i) = \emptyset V(\mu_i)$ 

where Ø is a dispersion parameter and is constant across the observations i

the linear predictor: 
$$g(\mu_i) = \eta_i$$

► a link function that describes how the mean, 
$$E(Y_i) = \mu_i$$
, depends on the linear predictor:

$$\eta_i = \beta_0 + \beta_1 x_{1i} + \dots + \beta_p x_{pi}$$

A generalized linear model is made up of a linear predictor:

# **Components of the GZLM**





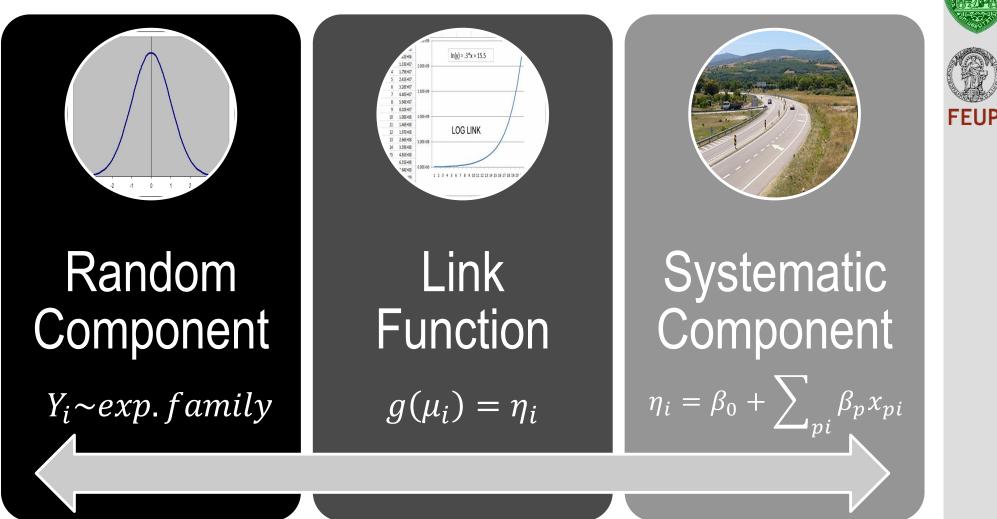
# Components of the GZLM

- $\Box$  Distribution of the Y's
  - > Linear models:  $Y_i \sim N(\mu_i, \sigma^2)$
  - $\succ$  GZLM:  $Y_i \sim exponential family$
- FEUP **Linear predictor =** function of the covariates (explanatory variables)
  - $\succ$  Linear models:  $\eta_i = \alpha + \beta x_i$
  - $\succ$  GZLM: e.g.  $\eta_i = \alpha + \beta x_i + \gamma z_i$  $\eta_i = \alpha + \beta x_i + \gamma x_i^2$

$$\Rightarrow \text{ Linear models:} \qquad n_i = \mu_i \Rightarrow \mu_i = \alpha + \beta x_i \qquad \text{Inverse function} \\ \Rightarrow \text{ GZLM:} \qquad e.g. \ \eta_i = \ln(\mu_i) \Rightarrow \mu_i = e^{(\alpha + \beta x_i + \gamma x_i^2)} \end{cases}$$

#### **Structure of Generalized Linear Models**





#### Fundamental condition for using GZLM

- Response variable distribution must be a member of the Exponential Family
  - > It corresponds to a <u>u</u> function that belongs to the exponential family with a single parameter  $\theta$  and a probability distribution function (pdf) such as

 $f(u, \theta) = s(u) \cdot t(\theta) \cdot \exp\{a(u) \cdot b(\theta)\}$ , where s, t, a, b are known functions

Or

 $f(u,\theta) = \exp\{a(u), b(\theta) + d(u) + c(\theta)\}$ 

where  $d(u) = \ln(s(u))$  and  $c(\theta) = \ln(t(\theta))$ 

- When a(u) = u, the distribution is said to be in canonical form.
  b(θ) is called the natural parameter of the distribution function.
- For each function of the Exponential Family, one **parameter is of interest**. The remaining are said **nuisance parameters**.

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#### Members of the Exponential Family: Normal Distribution

**D** Normal distribution: N( $\mu$ ,  $\sigma^2$ )

$$f(u,\mu) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot exp^{-\frac{1}{2}\left(\frac{u-\mu}{\sigma}\right)^2}, \text{ with } -\infty \le \mu \le \infty$$
Random Interest parameter
$$f(u,\mu) = exp\left\{u, \frac{\mu}{\sigma^2} + \left(\frac{-\mu^2}{2\sigma^2} - \frac{1}{2}\ln(2\pi\sigma^2)\right) - \left(\frac{-u^2}{2\sigma^2}\right)\right\}$$

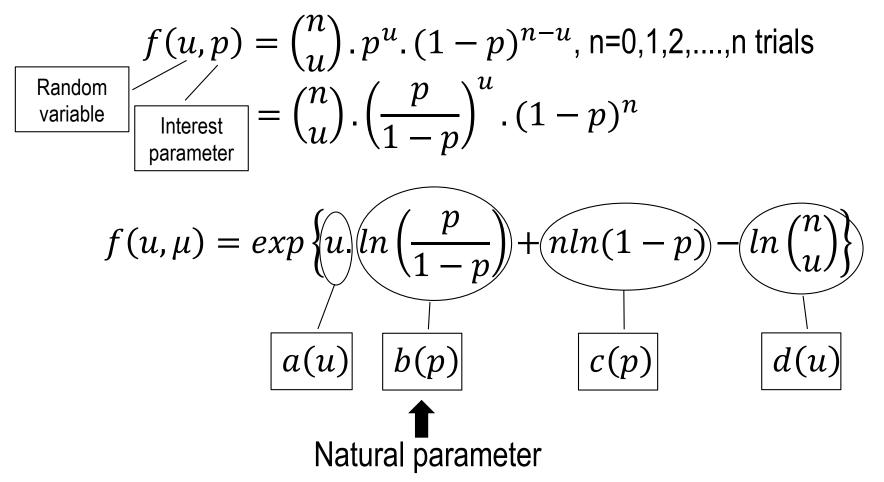
$$a(u) \quad b(\mu) \qquad c(\mu) \qquad d(u)$$
Natural parameter

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#### Members of the Exponential Family: Binomial Distribution

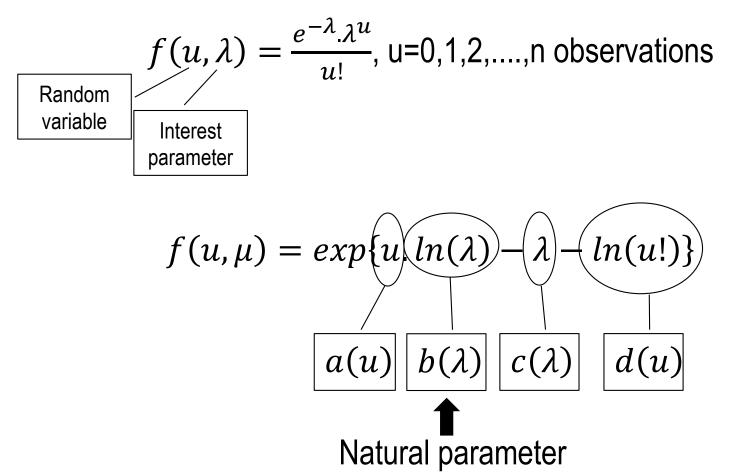
Binomial distribution: Bin(n, p)



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#### Members of the Exponential Family: Poisson Distribution

 $\square$  Poisson distribution: P( $\lambda$ )



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# Calibration of GZLM

□ Suppose we have a set of independent observations, where

>  $Y_i, X_i$ , for i=1,2,...n observations and  $X_i$  is a vector of regressors =  $X_1, X_2, ..., X_p$ and  $Y_i$  is a response variable (dependent variable) we want to estimate and that belongs to some Exponential Family



 $\succ$  The joint pdf can be written as:

$$f(Y_1, Y_2, ..., Y_n, \theta, \phi) = \prod_{i=1}^n exp\{Y_i, b(\theta_i) + c(\theta_i) + d(Y_i)\}$$
  
=  $exp\{\sum_{i=1}^n Y_i, \sum_{i=1}^n b(\theta_i) + \sum_{i=1}^n c(\theta_i) + \sum_{i=1}^n d(Y_i)\}$ 

- > The variation of Yi (through the link function) can be explained in terms of the regressors Xi, based on the calibrated coefficients  $\beta$
- > NOT THE VALUES OF YI THEMSELVES!!!!

distribution where a(Y)=Y

#### **Calibration of GZLM**



- **T** For  $X_i$ , a vector of regressors =  $X_1, X_2, \dots, X_p$ 
  - > We hope to find a set of parameters  $\beta = (\beta_1, \beta_2, ..., \beta_p)$  that fits the regressor values to a link function  $g(\mu_i)$  that transforms the response variable (Yi) such that, in the case of the normal distribution N( $\mu$ ,  $\sigma^2$ ),

$$E[\mu_i] = \mu_i = g(\mu_i) = BX$$
  
Link function

When the response variable Yi follows a normal distribution, the GZLM is equal to the MLR

$$E[Y_i] = \mu_{yi} = BX + E[\epsilon] = BX$$
, as  $E[\epsilon]=0$ 

# Calibrating regressions

**Maximum Likelihood Estimation (MLE) - Recap** 

#### **Obtain the likelihood**:

 $L(\mu) = f(y_1).f(y_2)...f(y_n)$ 

- □ Log it to make it easier to differentiate  $ln[L(\mu)]$
- □ Differentiate and set the derivative equal to zero:

$$\frac{\delta}{\delta\mu}(ln[L(\mu)]) = 0 \Rightarrow \hat{\mu} = \cdots$$

**Check its maximum:** 

$$\frac{\delta^2}{\delta\mu^2}(\ln[L(\mu)]) < 0 \Rightarrow max$$



#### Calibrating GLZM Maximum Likelihood Estimation (MLE)

#### **Obtain the likelihood**:

 $L(\mu_1, \mu_2, ..., \mu_n) = f(y_1).f(y_2)...f(y_n)$ 

- **Log it** to make it easier to differentiate  $ln[L(\mu_1, \mu_2, ..., \mu_n)]$
- □ Use the link function to replace the  $\mu'_i s$ :  $ln[L(\beta_1, \beta_2, \beta_3, ...)]$

□ Differentiate and set the derivative equal to zero:

$$\frac{\delta}{\delta\beta_1} (ln[L(\beta_1, \beta_2, \beta_3, \dots)]) = 0 \Rightarrow \widehat{\beta_1} = \cdots$$
$$\frac{\delta}{\delta\beta_2} (ln[L(\beta_1, \beta_2, \beta_3, \dots)]) = 0 \Rightarrow \widehat{\beta_2} = \cdots$$

□ Obtain the vector of  $\beta_i$  that fit the model estimates to the link function  $g(\mu_i)$ 

#### Link functions and Inverse functions

□ If the random component of *Yi* follows a **normal distribution** 

- > The corresponding **natural parameter** is:  $b(\mu_i) = \mu_i$
- > The link function is:  $g(\mu_i) = \mu_i$  (Identity link)
- > Then:  $g(\mu_i) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots = BX$
- > And inversely:  $\mu_i = BX$

□ If the random component of *Yi* follows a **binomial distribution** 

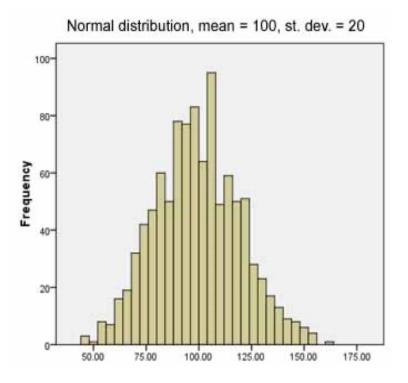
- > The corresponding natural parameter is:  $b(\mu_i) = ln\left(\frac{p_i}{1-p_i}\right)$
- > The link function is:  $g(\mu_i) = ln\left(\frac{p_i}{1-p_i}\right)$  (logit link or logistic)

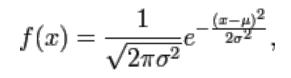
> Then: 
$$g(p_i) = ln\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots = BX$$

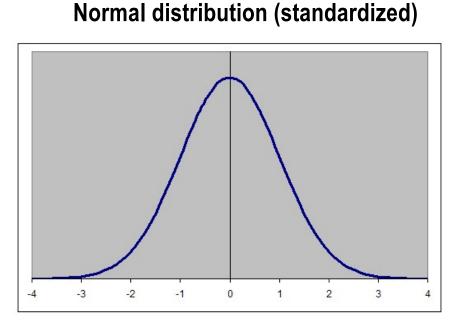
> And inversely: 
$$E[Y_i] = p_i = \frac{exp^{(BX)}}{1 + exp^{(BX)}}$$

#### Generalized Linear Models Normal distribution

- □ The distribution of the dependent variable has the form of the bellshaped symmetrical curve centered in the mean.
- □ This implies the dependent variable is continuous.



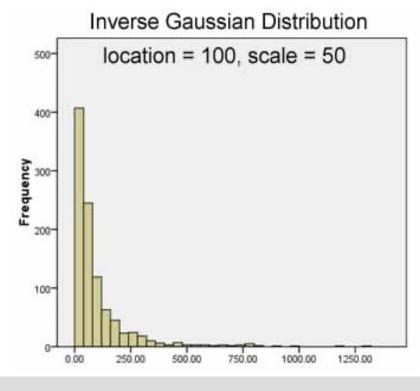




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### Generalized Linear Models Inverse Gaussian (Wald Distribution)

- □ It is used for dependent variables that are **positively skewed** and have values always greater than 0.
- Values must be greater than 0 or are dropped. It has been used to model diffusion processes, insurance claims, etc



If  $\lambda$  tends to infinity, the distribution becomes like a Normal distribution

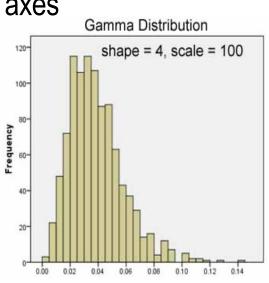
$$f(x;\mu,\lambda) = \left[\frac{\lambda}{2\pi x^3}\right]^{1/2} \exp \frac{-\lambda(x-\mu)^2}{2\mu^2 x}$$



#### Generalized Linear Models Gamma

- □ This is an alternative for positively skewed dependent variables. It is highly sensitive to the shape parameter.
  - When the shape parameter is greater than 1, the gamma distribution is bell-shaped but positively skewed as shown in the figure below.
  - When the shape parameter is 1, the gamma distribution is exponentially declining.
  - When the shape parameter is less than 1, the gamma distribution is also exponentially declining and asymptotic to the axes
- The gamma distribution has been used in survival analysis and modeling duration-of-event data.

$$f(x;k,\theta) = x^{k-1} \frac{e^{-x/\theta}}{\theta^k \Gamma(k)} \text{ for } x \ge 0 \text{ and } k, \theta > 0.$$







#### Generalized Linear Models Multinomial

This distribution is used when the dependent variable has a finite number of categories, such as text string values, or is ordinal.
 The distribution among categories, not shown, is arbitrary.

$$f(x_1,\ldots,x_k;n,p_1,\ldots,p_k) = \Pr(X_1 = x_1 \text{ and } \ldots \text{ and } X_k = x_k)$$

$$= egin{cases} rac{n!}{x_1!\cdots x_k!} p_1^{x_1}\cdots p_k^{x_k}, & ext{ when } \sum_{i=1}^k x_i = n \ 0 & ext{ otherwise,} \end{cases}$$





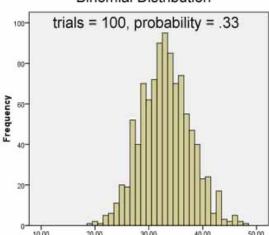
# Generalized Linear Models Binomial

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- □ Used when the **dependent variable is binary**.
- The count of events in a fixed number of trials also has a binary distribution. Examples of binomial data are attributes "present/not present", "innovation adopted/not adopted", or "success/failure" data.
- It is assumed that the two values have a fixed rather than changing probability of occurrence (as in coin-flipping), even if that probability Binomial Distribution
  Binomial Distribution

$$f(k; n, p) = \Pr(K = k) = \binom{n}{k} p^k (1 - p)^{n-k}$$

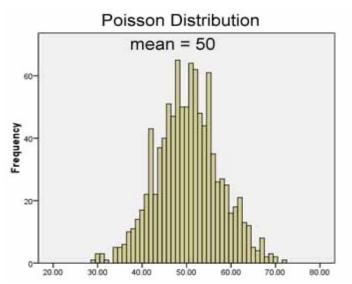
$$F(x;n,p) = \Pr(X \le x) = \sum_{i=0}^{\lfloor x \rfloor} \binom{n}{i} p^i (1-p)^{n-i}$$



#### Generalized Linear Models Poisson (COUNT DATA)

- The Poisson distribution is also used for count data and is preferred when events are rare, as in modeling accidents, wars, or epidemics
- The binomial distribution is used when the dependent variable corresponds to data counts of successes per given number of trials
- The Poisson distribution is used to count successes per given number of time units
  Poisson Distribution

$$f(k;\lambda) = \frac{\lambda^k e^{-\lambda}}{k!},$$





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### Generalized Linear Models Poisson (COUNT DATA)

- > A rule of thumb is to use a Poisson rather than binomial distribution when <u>n</u> is  $\geq$  100, the probability of each event is below 0.05
- The Poisson distribution is also used when "events" can be counted but non-occurrence of events cannot be counted (unreported).
- □ In Poisson distributions, the mean equals the variance
  - ➢ Presence of homoscedasticity since variance doesn't change over data and *λ* is assumed constant
  - > As such, there is **no over-dispersion of data**.
- □ All values are non-negative integers
  - Thus, count data, which cannot be negative, are better represented by Poisson than normal distributions

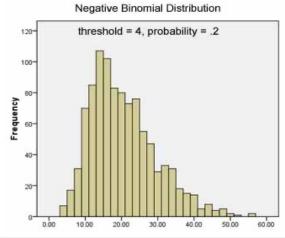


#### Generalized Linear Models Negative binomial

- □ It is like the Poisson distribution, also used for count data, but it is used when the variance is larger than the mean => over-dispersion of data.
- □ Typically, this is characterized by "there being too many 0's."
  - As such, not all cases have an equal probability of experiencing the rare event, but instead, events may be clustered.
  - The negative binomial model is therefore sometimes called the "over dispersed Poisson model". Values must still be non-negative integers.
- □ The negative binomial is specified by an ancillary /dispersion parameter k (sometimes referred to as  $\alpha$  or  $\psi$ ).
  - When k=0, the negative binomial is equal to the Poisson distribution.

$$f(k) \equiv \Pr(X=k) = \binom{k+r-1}{k} (1-p)^r p^k \quad \text{for } k = 0, 1, 2, \dots$$







#### Generalized Linear Models Systematic component

#### □ The linear predictor

- Quantity that incorporates the information about the independent variables into the model
- □ For a matrix of <u>n</u> observations and of <u>p</u> variables, the linear predictor <u>n</u> can be expressed as:

$$\eta_i = \sum_{j=1}^p x_{ij} \beta_j$$

□ Where

♦ each  $x_{ij}$  is the value of the j<sup>st</sup> IV for the i<sup>st</sup> observation

 $\boldsymbol{\ast} \boldsymbol{\beta}_{i}$  belong to a vector of unknown parameters to be estimated



It provides the relationship between the linear predictor and the mean of the distribution function

- > The way the two previous components relate to each other
- In fact, the link function is a transformation of the response variable

 $\Box$  It is a monotonous and differentiable function  $g(\mu_i)$  that transforms

 $\mu_i$  in  $\eta_i$  where  $g(\mu_i) = \eta_i$ 

 $\Box$  Inversely,  $\mu_i$  can be obtained with (inverse function)

$$E[Y_i] = \mu_i = g^{-1} (\beta_0 + \beta_1 X_{i1} + \dots + \beta_p X_{ip}) + e_i$$

where  $\mu_i$  is the expected value of  $Y_i$ and  $X_{ij}$  are the predictors or explanatory variables



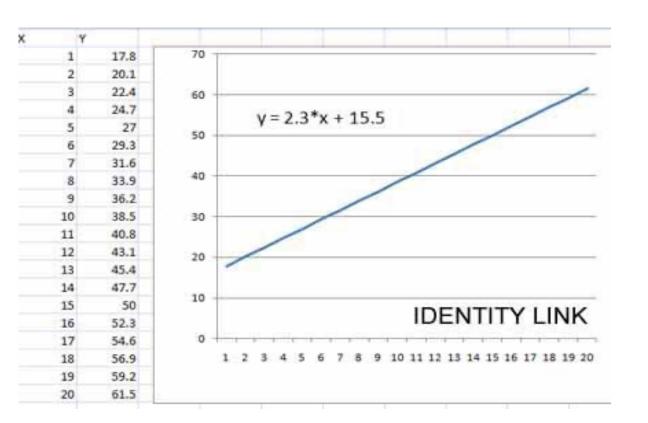


- It is used to maintain a linear relationship between the coefficients and predictors on the right-hand side of the model equation and the dependent variable transformed by the link function on the left-hand side of the equation
- The choices of the link function depend on the natural parameter of the original distribution of the dependent variable *Yi*



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#### □ Normal distribution: Identity function

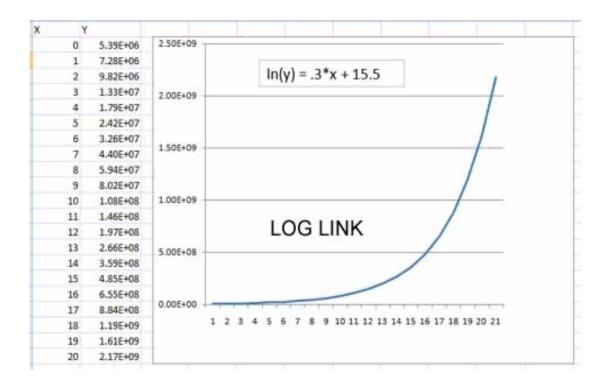


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- □ Poisson distribution: Log function
  - Loglinear models: assume a Poisson distribution and use a log link function





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#### □ Many other distributions: Power functions



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#### Common relations between distributions and link functions

Canonical Link Functions			
Distribution	Name	Link Function – $\eta_i 0 g(\mu_i)$	$\mu_i$ - Mean (Inverse) Function
Normal	Identity	$\mathbf{X}oldsymbol{eta}=\mu$	$\mu = \mathbf{X} oldsymbol{eta}$
Exponential	Inverse	$\mathbf{X}oldsymbol{eta} = \mu^{-1}$	$\mu = (\mathbf{X} \boldsymbol{eta})^{-1}$
Gamma	Inverse	Balling Profession	
Inverse	Inverse squared	$\mathbf{X}oldsymbol{eta}=\mu^{-2}$	$(\mathbf{v}_{0})^{-1/2}$
Gaussian	Inverse squared		$\mu = (\mathbf{X}\boldsymbol{\beta})^{-1/2}$
Poisson	Log	$\mathbf{X}oldsymbol{eta} = \ln{(\mu)}$	$\mu = \exp\left(\mathbf{X}\boldsymbol{eta} ight)$
Binomial	Logit	$\mathbf{X}\boldsymbol{\beta} = \ln\left(\frac{\mu}{1-\mu}\right)$	$\exp\left(\mathbf{X}\boldsymbol{\beta}\right) = 1$
Multinomial	Logit	$(1-\mu)$	$\mu = \frac{\exp\left(\mathbf{X}\boldsymbol{\beta}\right)}{1 + \exp\left(\mathbf{X}\boldsymbol{\beta}\right)} = \frac{1}{1 + \exp\left(-\mathbf{X}\boldsymbol{\beta}\right)}$



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- The Poisson Distribution is commonly used to describe the count of events occurring at random in time or space
- **The Poisson condition is that**  $E[Y_i] = VAR[Y_i] = \lambda_i$  or that

□ Examples:

- The number of cars passing through an intersection during a certain hour
- The number of calls for emergency ambulance service during a tour of duty
- The number of fires arising in a neighborhood
- Number of vehicles waiting in a queue
- ✤ Auto breakdowns in an express way in rush hour
- Number of heart attack deaths per week in a county
- Number of homes destroyed by a fire during the summer
- Number of accidents in a road section or intersection

The most common relationship between the explanatory and the Poisson parameter is the log-linear model (because the logarithm of this function produces the linear combination of explanatory variables)



**Inverse function** 

$$\lambda_{i} = e^{(\beta Xi)}$$
or
$$E[Yi] = \lambda_{i} = \exp\left(\beta_{0} + \sum_{j=1}^{p} x_{ij}\beta\right)$$

$$Ln(\lambda_{i}) = \beta Xi$$

The expected number of accidents per period is given by

$$E[y_i] = \lambda_i = e^{(\beta X_i)}$$

#### Poisson model

- For the case of count data (e.g., accidents), a variable Q<sub>i</sub> is added and corresponds to the unit of exposure (e.g., vehicles per year)
- > It is also referred to as the offset value

$$E[Y_i] = Q_i \times exp\left(\beta_0 + \sum_{j=1}^p x_{ij}\beta_j\right)$$



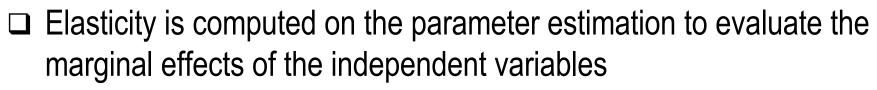
Estimation by standard maximum likelihood methods, with the likelihood function given as

$$L(\beta) = \prod \frac{EXP[EXP(\beta X_i)][EXP(\beta X_i)]^{y_i}}{y_i!}$$

Oľ

$$LL(\beta) = \sum_{i=1}^{n} \left[-EXP(\beta X_i) + y_i \beta X_i - LN(y_i!)\right]$$

Maximum likelihood estimates produce Poisson parameters witch are consistent, asymptotically normal, and asymptotically efficient



- > Effect of a 1% change in the variable on the expected frequency  $\lambda_i$
- Computed for each observation and then a single average is reported
- Continuous variables

$$E_{x_{ik}}^{\lambda_i} = \frac{\delta \lambda_i}{\lambda_i} \times \frac{x_{ik}}{\delta x_{ik}} = \beta_k x_{ik}$$

Count data

$$E_{xik}^{\lambda i} = \frac{EXP(\beta_k) - 1}{EXP(\beta_k)}$$



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# GZLM for count of events Negative Binomial Regression

- □ When the Poisson condition is violated (i.e.,  $E[Y_i] \neq VAR[Y_i]$ ), two situations can occur:
  - $E[Y_i] > VAR[Y_i]$  (dispersed)
  - $E[Y_i] < VAR[Y_i]$  (over dispersed)
- $\hfill\square$  As such, the link function is rewritten
  - from  $\lambda_i = EXP(\beta Xi)$  for each observation , with

 $\lambda_i = EXP(\beta Xi + \varepsilon i)$ 

 $\succ$  where  $\epsilon_{i}$  is the dispersion term



# GZLM for count of events Negative Binomial Regression





Therefore the variance differ from the mean through the addition of a quadratic term to the variance that represents over dispersion

 $\operatorname{var}(Y_i) = \lambda_i + K(\lambda_i)^2$ 

- The Poisson model is regarded as a limited model of the negative binomial as K approaches 0.
- □ This K parameter is called the **over dispersion** parameter.

# GZLM for count of events Negative Binomial Regression- MLE

□ Negative Binomial pdf

$$P(y_i) = \frac{\Gamma\left(y_i + \frac{1}{K}\right)}{y_i!\Gamma\frac{1}{K}} \left(\frac{K\lambda_i}{(1 + K\lambda_i)}\right)^{y_i} \left(\frac{1}{1 + K\lambda_i}\right)^{\frac{1}{K}}$$

- where Γ is a Gamma Function and K is an estimated parameter representative of dispersion
- □ The corresponding likelihood function is:

$$L(\lambda_i) = \prod \frac{\Gamma\left(y_i + \frac{1}{K}\right)}{y_i! \Gamma \frac{1}{K}} \left(\frac{K\lambda_i}{(1 + K\lambda_i)}\right)^{y_i} \left(\frac{1}{1 + K\lambda_i}\right)^{\frac{1}{K}}$$

# GZLM for count of events Negative Binomial Regression

□ Negative Binomial with log link



- Specifies a negative binomial distribution (with the ancillary K parameter = 1) with a log link function
  - It is used to modeling count data that violates the Poisson assumption of equality of mean and variance.
  - Also, negative binomial regression is thought to be more stable than Poisson regression for small datasets.
  - > An error term  $\xi$  of Gamma distribution and variance  $K_2$  is added to the Poisson Regression

$$\log(\lambda_i) = \beta_0 + \sum_{j=1}^p x_{ij}\beta_j + \xi_i$$

# GZLM for count of events Negative Binomial Regression

□ Tests on over dispersion - Lagrange Multiplier test (in SPSS)

- The Lagrange multiplier test may be used to test if a negative binomial model is significantly different from a Poisson model
- Since the negative binomial model is the same as the Poisson model when the binomial model's ancillary (dispersion) parameter, K=0, the Lagrange multiplier test analyses the null hypothesis that K = 0
- A significant Lagrange test coefficient (i.e., *p-value* > 0,05) indicates that *K* cannot be assumed to be different from 0, and hence a Poisson model would be preferred over a negative binomial model (negative binomial models have one more parameter, *k*)



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