# COMP 680 Statistics for Computing and Data Science Week 12: Generalized Linear Models

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## Outline

**GLM Family** 

- GLM Family
- 2 Logistic Regression
- Multinomial Regression
- Poisson Regression
- 6 Advanced Topics
- Code Demo



Week 12

## Generalized Linear Models

**GLM Family** 

- A large class of models!
  - where the error distribution is no longer restricted to be Gaussian



## Generalized Linear Models

**GLM Family** 

- A large class of models!
  - where the error distribution is no longer restricted to be Gaussian
- The conditional distribution of Y|X follows exponential family
  - linear regression is one type of GLM
    - exponential family: Gaussian, Binomial, Poisson, Gamma, Beta ...



## Generalized Linear Models

**GLM Family** 

- A large class of models!
  - where the error distribution is no longer restricted to be Gaussian
- The conditional distribution of Y|X follows exponential family
  - linear regression is one type of GLM
  - exponential family: Gaussian, Binomial, Poisson, Gamma, Beta ...
- Model the conditional mean of Y|X
  - $\mathbb{E}[Y|X] = X\beta$  for LM
  - $g(\mathbb{E}[Y|X]) = X\beta$  for GLM
  - different link functions g for specific conditional distributions

## LM as GLM

**GLM Family** 

A generalized linear model to model conditional mean  $\mu = \mathbb{E}[Y|X]$ :

$$g(\mu) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$



## LM as GLM

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#### GLM

- ullet a link function  $g(\mu)$ 
  - describes how the transformed mean depends on the linear predictor
- a variance function  $\phi V(\mu)$ 
  - how the variance of Y depends on the mean  $\mu$  where  $\phi$  is the dispersion parameter

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#### LM (a special case)

- $g(\mu) = \mu$ 
  - link function for LM is the identity function, i.e. no transformation needed
- $V(\mu) = 1$ 
  - for Gaussian distribution. variance does not depend on mean, and  $\phi = \sigma^2$

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## Link Functions

**GLM Family** 

Response Y	Conditional Distribution	Link Function
Continuous	Gaussian	Identity function
Continuous	Gamma	Negative inverse function
Continuous	Inverse Gaussian	Inverse squared function
Binary	Binomial	Logit function
Categorical	Multinomial	(generalized) Logit function
Ordinal	Multinomial	Logit or Probit function
Count	Poisson	Log function
Count	Negative Binomial	Log function

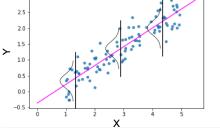


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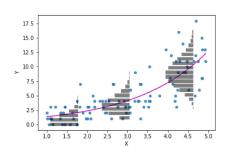
## Illustration

**GLM Family** 

Linear regression



Poisson regression



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## Binary Outcome

- Examples of binary responses
  - spam filter
  - fraud detection
  - cancer screening
  - ..



## Binary Outcome

- Examples of binary responses
  - spam filter
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  - cancer screening
  - ..
- In Machine Learning: Binary Classification



Logistic Regression Multinomial Regression Poisson Regression Advanced Topics Code Demo

## Binary Outcome

- Examples of binary responses
  - spam filter
  - fraud detection
  - cancer screening
  - ..
- In Machine Learning: Binary Classification
  - a type of supervised learning
  - Logistic Regression is one classifier
  - many others: KNN, NaiveBayes, DecisionTrees, SVM, ...

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#### Bernoulli and Binomial Distributions

- A Bernoulli random variable Y is a discrete random variable that can only take values 0 or 1:
  - a single parameter p: "success" probability
  - $\mathbb{P}(Y = 1) = p$ : "success"
  - $\mathbb{P}(Y = 0) = 1 p$ : "failure"
  - $\mathbb{E}[Y] = p$ , var(Y) = p(1-p)



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  - $\mathbb{E}[Y] = p$ , var(Y) = p(1-p)
- A Binomial random variable Y is the sum of n independent Bernoulli's:
  - two parameters: n and p
  - Y is a discrete random variable and can take values from 0 to n
  - $\mathbb{P}(Y = k) = \binom{n}{k} p^k (1-p)^{n-k}$ : k "success" out of n trials
  - $\mathbb{E}[Y] = np$ , var(Y) = np(1-p)

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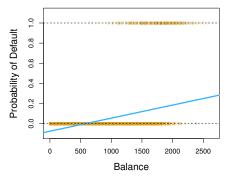
## Linear vs. Logistic Regression

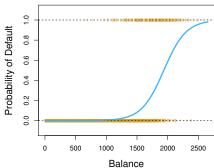
Why not linear regression, model  $\mathbb{E}[Y|X] = p_x$  with a straight line?



## Linear vs. Logistic Regression

Why not linear regression, model  $\mathbb{E}[Y|X] = p_X$  with a straight line?





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#### The logit function:

- $logit(x) = ln\left(\frac{x}{1-x}\right)$
- log odds ratio

## The logistic function:

- $f(x) = \frac{e^x}{1+e^x}$
- Sigmoid function



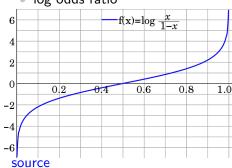
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## Logit and Logistic

#### The logit function:

• 
$$logit(x) = ln\left(\frac{x}{1-x}\right)$$

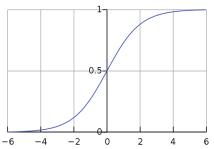
log odds ratio



#### The logistic function:

• 
$$f(x) = \frac{e^x}{1+e^x}$$

Sigmoid function



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## Simple Logistic Model

$$\mathbb{P}(Y=1|X) = p_{\scriptscriptstyle X} = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}} \Leftrightarrow \mathsf{logit}(p_{\scriptscriptstyle X}) = \mathsf{ln}\left(\frac{p_{\scriptscriptstyle X}}{1 - p_{\scriptscriptstyle X}}\right) = \beta_0 + \beta_1 x$$



$$\mathbb{P}(Y=1|X) = p_{\scriptscriptstyle X} = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}} \Leftrightarrow \mathsf{logit}(p_{\scriptscriptstyle X}) = \mathsf{ln}\left(\frac{p_{\scriptscriptstyle X}}{1 - p_{\scriptscriptstyle X}}\right) = \beta_0 + \beta_1 x$$

- remember  $\mu = \mathbb{E}[Y|X] = p_{\mathsf{x}}$  for binary Y
- the link function  $g(\mu)$  is the logit function
- log odds ratio is a linear function of X!

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- How to estimate model parameters: Maximum Likelihood Estimate
  - likelihood function?



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- Point estimate for model coefficients: \(\hat{\beta}\_0\) and \(\hat{\beta}\_1\)
  - can make inference
    - asymptotic normality of MLE



- How to estimate model parameters: Maximum Likelihood Estimate
  - likelihood function?
- Unlike linear models, does not have closed form solutions
  - numerical optimization Newton's method
- Point estimate for model coefficients:  $\hat{eta}_0$  and  $\hat{eta}_1$ 
  - can make inference
    - asymptotic normality of MLE
  - can make prediction
    - predict log odds  $\rightarrow$  probability  $\rightarrow$  label

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## Model Interpretation

#### Linear Regression:

- $\hat{y} = \hat{\beta_0} + \hat{\beta_1} x$
- $\hat{\beta}_0$ : average value of Y when X=0
- $\hat{\beta}_1$ : average change in Y when X increase by 1 unit
- $\hat{\beta}_1 > 0$  and significant: X is positively correlated with Y



#### Linear Regression:

- $\hat{\mathbf{v}} = \hat{\beta}_0 + \hat{\beta}_1 \mathbf{x}$
- $\hat{\beta}_0$ : average value of Y when X = 0
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#### Logistic Regression

- $\ln\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{\beta}_0 + \hat{\beta}_1 x$
- $\hat{\beta}_0$ : log odds of Y=1 when X = 0
- $\hat{\beta}_1$ : change in log odds of Y=1when X increase by 1 unit
- $\hat{\beta}_1 > 0$  and significant: X is positively correlated with log odds of Y=1



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## Multiple Covariates

- ullet simple linear regression o multiple regression
  - interpretation of single slope means controlling others



## Multiple Covariates

- simple linear regression → multiple regression
  - interpretation of single slope means controlling others
- ullet simple logistic regression o multiple logistic regression
  - A set of p covariates  $X_1, X_2, \cdots X_p$

$$\mathbb{P}(Y=1|X) = p_{X} = \frac{e^{\beta_{0} + \beta_{1}X_{1} + \dots + \beta_{p}X_{p}}}{1 + e^{\beta_{0} + \beta_{1}X_{1} + \dots + \beta_{p}X_{p}}} \Leftrightarrow \log_{\mathbf{r}}(p_{X}) = \ln\left(\frac{p_{X}}{1 - p_{X}}\right) = \beta_{0} + \beta_{1}X_{1} + \dots + \beta_{p}X_{p}$$

 interpretation of single slope means controlling others (holding others constant), exactly the same!

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- From predicted probability  $\hat{p} = \mathbb{P}(\hat{Y} = 1)$  to predicted outcome  $\hat{Y}$ 
  - a natural threshold 0.5
  - $\hat{p} = \mathbb{P}(\hat{Y} = 1) \ge 0.5 \Rightarrow \hat{Y} = 1$   $\hat{p} = \mathbb{P}(\hat{Y} = 1) < 0.5 \Rightarrow \hat{Y} = 0$



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Pearson residue

$$rac{y_i - \hat{p}_i}{\sqrt{\hat{p}_i(1-\hat{p}_i)}}$$



#### Prediction

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Pearson residue

$$\frac{y_i - \hat{p}_i}{\sqrt{\hat{p}_i(1-\hat{p}_i)}}$$

- Can vary threshold to minimize error measure
  - sensitivity: true positive rate
  - specificity: true negative rate



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## Categorical Outcome

- More than 2 outcomes
  - multi-class classification



## Categorical Outcome

- More than 2 outcomes
  - multi-class classification
- Multinomial regression
  - extension on logistic regression
  - multi-class logistic regression



- A Multinomial random variable (vector)  $Y = (Y_1, \dots, Y_K)$ 
  - K parameters: n and probabilities  $(p_1, p_2, \cdots p_K)$
  - $\sum_{k=1}^{K} p_k = 1$
  - Y represents number of k different outcomes



- A Multinomial random variable (vector)  $Y = (Y_1, \dots Y_K)$ 
  - K parameters: n and probabilities  $(p_1, p_2, \cdots p_K)$
  - $\sum_{k=1}^{K} p_k = 1$
  - Y represents number of k different outcomes
- A Binomial is a special case of Multinomial where K=2
  - $(p_1 = p, p_2 = 1 p)$



### Generalized Logit

You have total of K categories, pick a category to be baseline

$$\mathbb{P}(Y=j|X) = 
ho_{x}^{j} = rac{e^{eta_{0}^{j} + eta_{1}^{j} X_{1} + \cdots + eta_{p}^{j} X_{p}}}{1 + \sum_{k=1}^{K-1} e^{eta_{0}^{k} + eta_{1}^{k} X_{1} + \cdots + eta_{p}^{k} X_{p}}}, \quad j=1,\cdots K-1$$



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- K-1 set of p+1 parameters to estimate
- Softmax function

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### Generalized Logit

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- K-1 set of p+1 parameters to estimate
- Softmax function
- which one to be your baseline DOES NOT matter
- interpretation of coefficients: odds of category j vs. baseline
- Binary Logistic is a special case of K=2 and Y=0 as baseline

#### Ordinal Outcome

- Ignore ordinal information and use Multinomial Regression
  - less efficient, (K-1)(p+1) parameters



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- Ignore ordinal information and use Multinomial Regression
  - less efficient, (K-1)(p+1) parameters
- Use ordinal information
  - more efficient, K + p 1 parameters
- Intuition
  - unlike multinomial case, now the categories are ordered
  - the difference between category k-1 and k should be comparable to the difference between category k and k+1

### Ordinal Logistic Regression

The Proportional-Odds Cumulative Logit Model

$$\log\left(\frac{\mathbb{P}(Y \leq k|X)}{1 - \mathbb{P}(Y \leq k|X)}\right) = \beta_0^k + \beta_1 X_1 + \cdots + \beta_p X_p, \quad k = 1, 2, \cdots K - 1$$

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### Ordinal Logistic Regression

• The Proportional-Odds Cumulative Logit Model

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• estimate K-1 intercept and p slopes



### Ordinal Logistic Regression

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- estimate K-1 intercept and p slopes
- Interpretation of coefficients:
  - $\beta_0^k$  is the log odds of falling into or below category k when all X=0
  - $\beta_j$  is increase in log odds of falling into or below any category associated with a one unit increase in  $X_i$  while controlling all other X

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#### Poisson Distribution

• A Poisson random variable X is discrete and can take any integer values with single parameter  $\lambda$ :

$$\mathbb{P}(X=k) = \frac{\lambda^k e^{-\lambda}}{k!}$$



#### Poisson Distribution

• A Poisson random variable X is discrete and can take any integer values with single parameter  $\lambda$ :

$$\mathbb{P}(X=k)=\frac{\lambda^k e^{-\lambda}}{k!}$$

• 
$$\mathbb{E}[Y] = \text{Var}(Y) = \lambda$$



## Poisson Regression

Link function is natural log

$$\log(\mathbb{E}[Y|X]) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$



### Poisson Regression

Link function is natural log

$$\log(\mathbb{E}[Y|X]) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

- Interpretation of slopes:
  - one unit increase of  $X_j$  impacts average value of Y by multiplication of  $e^{\beta_j}$  while holding all other X constant

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#### Poisson GLM for Rates

- Response Y has a Poisson distribution, and t is index of the time (or space).
  - count of incidents during specific period of time



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$$\log(\mathbb{E}[Y]/t) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

- the term log(t) is referred to as an offset, an adjustment term
- the mean count is proportional to t

### Overdispersion

- In practice, the apparent variance of data often exceeds the mean, reflecting overdispersion in the model parameters.
  - cause covariates to be "more significant"
  - narrower confidence intervals than warranted by the data



### Overdispersion

- In practice, the apparent variance of data often exceeds the mean, reflecting overdispersion in the model parameters.
  - cause covariates to be "more significant"
  - narrower confidence intervals than warranted by the data
- Possible solutions
  - quasi-Poisson or negative binomial generalized linear model
  - more parameter and no longer force mean = variance



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# **Exponential Family**

 A single-parameter exponential family PDF (or PMF) can be expressed in the form:

$$f_X(x \mid \theta) = h(x) \exp[\eta(\theta) \cdot T(x) + A(\theta)]$$



# **Exponential Family**

 A single-parameter exponential family PDF (or PMF) can be expressed in the form:

$$f_X(x \mid \theta) = h(x) \exp[\eta(\theta) \cdot T(x) + A(\theta)]$$

- $\eta(\theta)$  is called the natural parameterization and is the link function!
  - each exponential distribution corresponds to a GLM
  - logistic and Poisson are most common

40 × 40 × 45 × 45 × 5 × 900

General:

$$f_X(x \mid \theta) = h(x) \exp[\eta(\theta) \cdot T(x) + A(\theta)]$$



### **Exponential Family**

General:

$$f_X(x \mid \theta) = h(x) \exp[\eta(\theta) \cdot T(x) + A(\theta)]$$

Binomial:

$$\mathbb{P}(X = x \mid p) = \binom{n}{k} p^{x} (1 - p)^{n - x}$$
$$= \binom{n}{k} \exp \left[ x \ln \left( \frac{p}{1 - p} \right) + n \ln(1 - p) \right]$$



# **Exponential Family**

• General:

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$$= \binom{n}{k} \exp \left[ x \ln \left( \frac{p}{1 - p} \right) + n \ln(1 - p) \right]$$

Poisson

$$\mathbb{P}(X = x \mid \lambda) = \frac{e^{-\lambda} \lambda^{x}}{x!} = \frac{1}{x!} \exp[x \ln \lambda - \lambda]$$

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• What is the goodness-of-fit measure in linear models?



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  - residual sum of squares (RSS)
  - $R^2$  and adjusted  $R^2$



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- ullet The notion of deviances: pprox 2log likelihood, smaller o better fit.



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  - R<sup>2</sup> and adjusted R<sup>2</sup>
- The notion of deviances: pprox 2log likelihood, smaller o better fit.
- Software output usually includes:
  - the null deviance shows how well the response variable is predicted by a model that includes only the intercept (grand mean).
  - the residual deviance can be compared to the null deviance:



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- Software output usually includes:
  - the null deviance shows how well the response variable is predicted by a model that includes only the intercept (grand mean).
  - the residual deviance can be compared to the null deviance:
- Akaike Information Criterion (AIC):
  - based on deviance, but penalize on model size
  - more useful in model comparison



Can compare AIC and choose the one with smaller AIC



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- Can perform hypothesis test
  - Hosmer-Lemeshow Goodness of Fit for binary response
  - in R package "ResourceSelection"
  - significant results means poor model fit



- Can compare AIC and choose the one with smaller AIC
- Can perform hypothesis test
  - Hosmer-Lemeshow Goodness of Fit for binary response
  - in R package "ResourceSelection"
  - significant results means poor model fit
- In general, GLM are estimated by MLE
  - Likelihood ratio test ( $\chi^2$  test)
  - significant results means larger model provide significant improvement

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