

Lecture 3: Binary and binomial regression models

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Overview

- Model classes for binary/binomial regression data
- Explorative data analysis (EDA) for binomial regression data
 - main effects
 - interaction effects

Binary regression models

Data: $(Y_i, \mathbf{x}_i) i = 1, \dots, n$ Y_i independent
 $Y_i = 1$ or 0
 $\mathbf{x}_i \in \mathbb{R}^p$ covariates (known)

Model: $p(\mathbf{x}_i) := P(Y_i = 1 | \mathbf{X}_i = \mathbf{x}_i)$
 $\Rightarrow P(Y_i = 0 | \mathbf{X}_i = \mathbf{x}_i) = 1 - p(\mathbf{x}_i)$

How to specify $p(\mathbf{x}_i)$? We need $p(\mathbf{x}_i) \in [0, 1]$.

Example: Survival on the Titanic

Source: <http://www.encyclopedia-titanica.org/>

Name Passenger Name

PClass Passenger Class

Age Age of Passenger

Sex Gender of Passenger

Survived Survived=1 means Passenger survived

Survived=0 means Passenger did not survive

Model hierarchy

Model 1) $p(\mathbf{x}) = F(\mathbf{x}) \quad F \in \{\textcolor{red}{F} : \mathbb{R}^p \rightarrow [0, 1]\}, F \text{ unknown}$

Model 2) $p(\mathbf{x}) = F(\mathbf{x}_i^t \boldsymbol{\beta}) \quad F \in \{\textcolor{red}{F} : \mathbb{R} \rightarrow [0, 1]\}, F \text{ unknown}$

Model 3) $p(\mathbf{x}) = F(\mathbf{x}_i^t \boldsymbol{\beta}) \quad F \in \{F : \mathbb{R} \rightarrow [0, 1] \text{ } \textcolor{red}{cdf}\}, F \text{ unknown}$

Model 4) $p(\mathbf{x}) = F_0(\mathbf{x}_i^t \boldsymbol{\beta}) \quad \textcolor{red}{F_0 \text{ known cdf}}$

Model properties

Model 1: - simple interpretation of covariate effects not possible
- estimation of p -dimensional F difficult
 → smoothing methods
 (O'Sullivan, Yandell, and Raynor (1986), Hastie and Tibshirani (1999))

Model 2: - estimation of F now one dimensional, but additional estimation for β needed
- Interpretation of covariate effects remains difficult

Model 3: - Since cdf 's are monotone, covariate effects are easily interpretable
- Different classes for cdf 's F can be chosen:

Parametric Approach: Link Families

$$\mathcal{F} = \{F(\cdot, \psi), \psi \in \Psi, F(\cdot, \psi) \text{ cdf}, F(\cdot, \cdot) \text{ known}\}$$

- ψ link parameter
- joint estimation of β and ψ is needed

Example:

(Czado 1997)

$$F(\eta, \psi) = \frac{e^{h(\eta, \psi)}}{1 + e^{h(\eta, \psi)}}$$

$$h(\eta, \psi) = \begin{cases} \frac{(\eta+1)^{\psi_1}-1}{\psi_1} & \eta \geq 0 \\ -\frac{(-\eta+1)^{\psi_2}-1}{\psi_2} & \eta < 0 \end{cases} \quad \psi = (\psi_1, \psi_2)$$

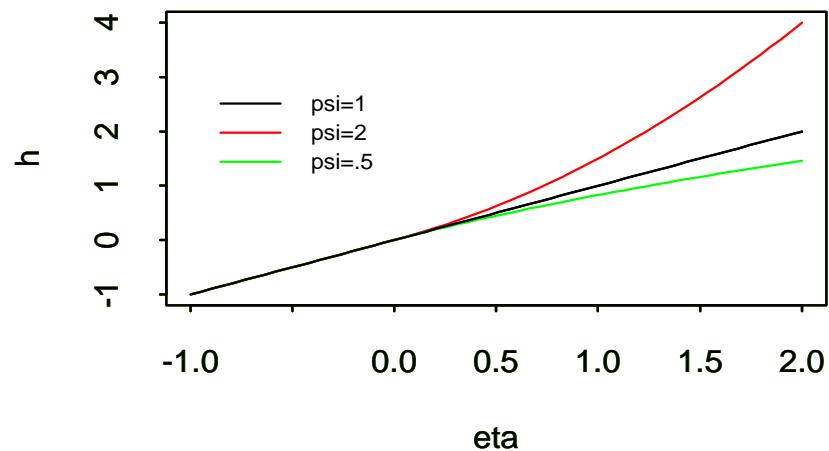
Both tail family

$\psi = (1, 1)$ corresponds to logistic regression

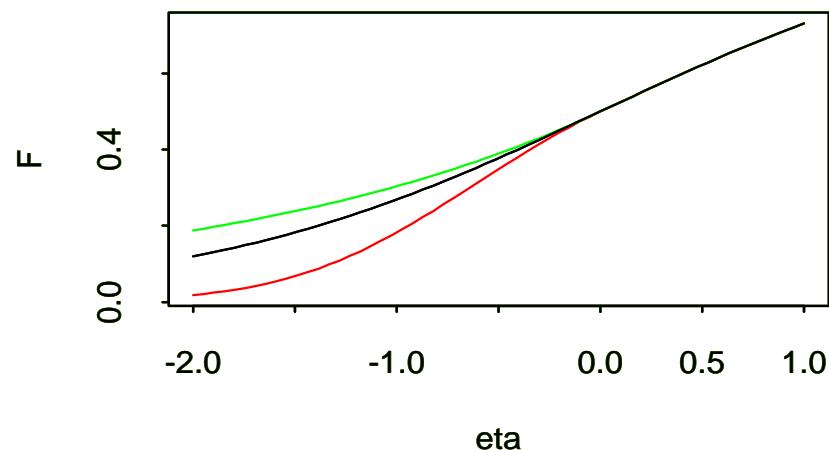
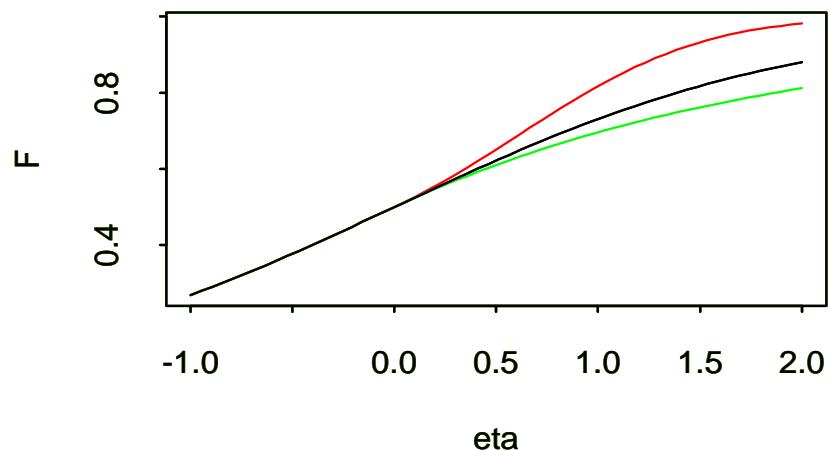
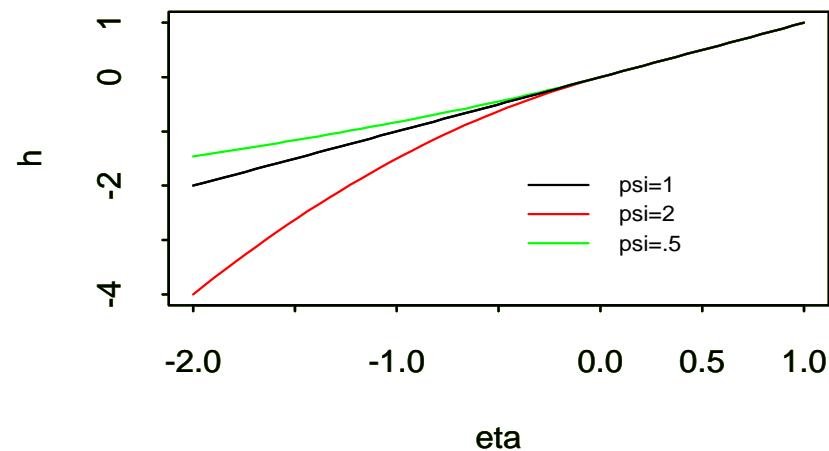
$\psi = (\psi_1, 1)$ Right tail family

$\psi = (1, \psi_2)$ Left tail family

Right Tail Modification



Left Tail Modification



Nonparametric Approach

- Klein and Spady (1993)
- Bayesian approach: need a prior for the class of *cdf*'s, i.e. a stochastic process such as the Dirichlet process. Markov Chain Monte Carlo (MCMC) methods are required to estimate the posterior distribution (see Newton, Czado, and Chappell (1996))

Restriction to *cdf*'s can be justified by the threshold approach:

$$Y_i = 1 \Leftrightarrow \mathbf{x}_i^t \boldsymbol{\beta} \geq U_i \quad \text{where } U_i \sim F \text{ i.i.d.}$$

$$\Rightarrow P(Y_i | \mathbf{X}_i = \mathbf{x}_i) = P(U_i \leq \mathbf{x}_i^t \boldsymbol{\beta}) = F(\mathbf{x}_i^t \boldsymbol{\beta})$$

Model 4:

- Most common and simplest model, however gives not always the best fit (link misspecification)

- Examples:

- $F(\eta) = \frac{e^\eta}{1+e^\eta}$ logistic regression
- $F(\eta) = \Phi(\eta)$ probit regression
- $F(\eta) = 1 - \exp\{-\exp\{\eta\}\}$ complementary log-log regression

Logistic regression

$Y_i | \mathbf{X}_i = \mathbf{x}_i \sim \text{binary}(p(\mathbf{x}_i))$ independent

$$p(\mathbf{x}_i) = P(Y_i = 1 | \mathbf{X}_i = \mathbf{x}_i) = \frac{e^{\mathbf{x}_i^t \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i^t \boldsymbol{\beta}}}$$

Binary response can be extended to binomial response:

$$\begin{aligned} Y_i &\sim \text{bin}(n_i, p(\mathbf{x}_i)) \text{ ind.} \\ \Rightarrow P(Y_i = y_i | \mathbf{X}_i = \mathbf{x}_i) &= \binom{n_i}{y_i} p(\mathbf{x}_i)^{y_i} (1 - p(\mathbf{x}_i))^{n_i - y_i}, \end{aligned}$$

i.e. $\left\{ \frac{Y_i}{n_i} \right\}$ is a GLM with canonical link.

Explorative data analysis (EDA) for binomial regression data

Data: (Y_i, \mathbf{x}_i) , $\mathbf{x}_i = (x_{i1}, \dots, x_{ik})$ k potentially important covariates.

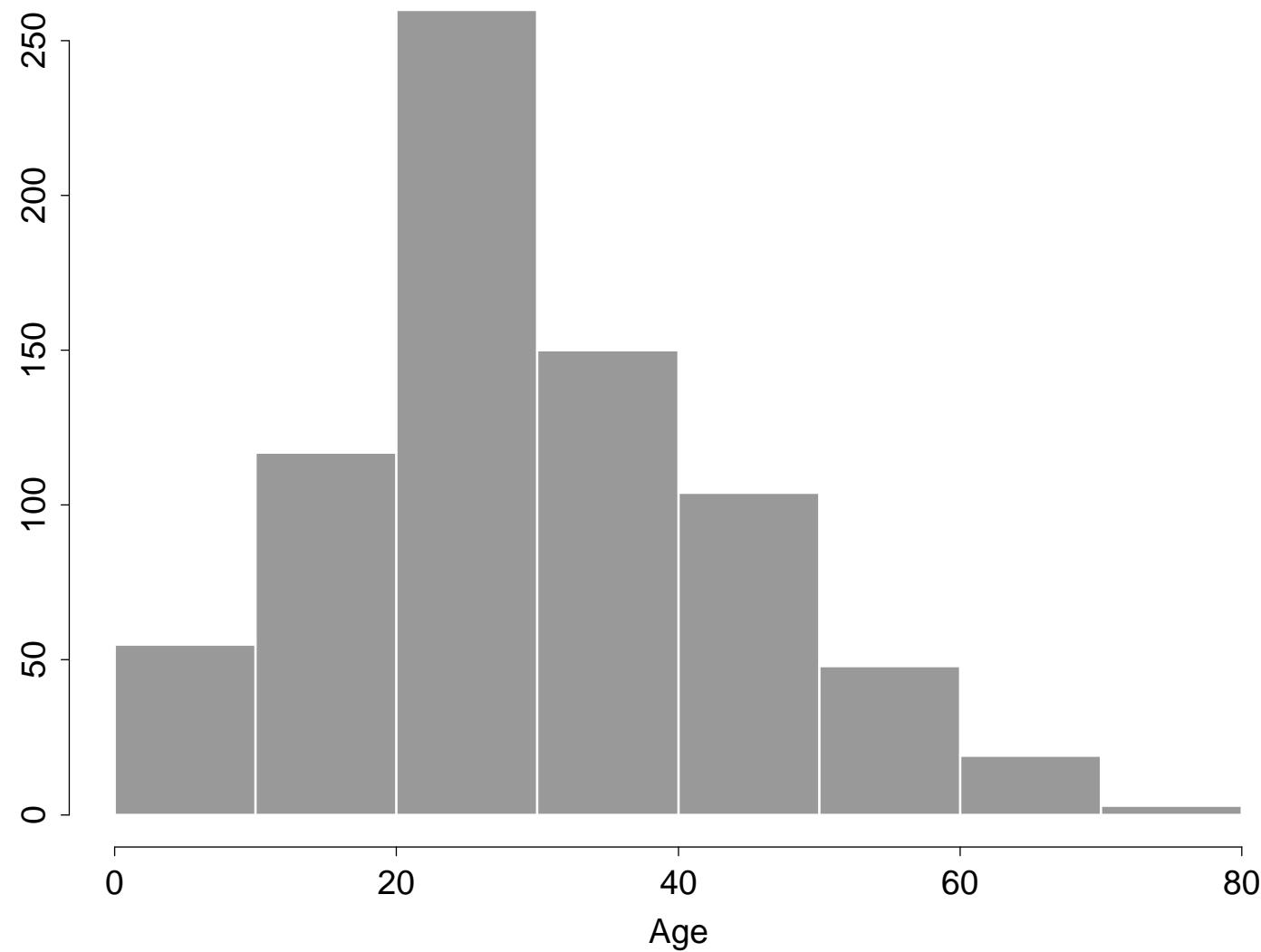
Problem: Variable selection.

With many covariates one needs screening methods, such as EDA.

covariates	qualitative / categorical	dichotomous	(2 levels)
		polytomous	(J levels)
		ordinal	(J levels)
	quantitative		

Example: Titanic data summaries

```
> attach(titanic)
> table(PClass)
  1st 2nd 3rd
  322 280 711
> table(Sex)
 female male
  462  851
> table(Survived)
   0   1
 863 450
```



```
> table(Survived,PClass)
  1st 2nd 3rd
0 129 161 573
1 193 119 138
> table(Survived,Sex)
  female male
0      154  709
1      308  142
```

Third Class and male passengers survived less often than other class or female passengers.

Influence of single covariate on $p(x)$

Dichotomous covariate.

Data

Status	Gender	
	female	male
not survived	154	709
survived	308	142

Want to estimate

Y	X	
	0	1
0	$1 - p(0)$	$1 - p(1)$
1	$p(0)$	$p(1)$

Logistic model: $p(x) = P(Y = 1|X = x) = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}}$ $x = 0, 1$

$o := \frac{p}{1-p}$ “odds of success”, p = success probability

$$\text{logit}(p) := \log(o) = \log\left(\frac{p}{1-p}\right) \text{ Log odds}$$

Influence of single covariate on $p(\mathbf{x})$

$$\left. \begin{aligned} logit(p(1)) &= \log \left(\frac{e^{\beta_0 + \beta_1 x} / (1 + e^{\beta_0 + \beta_1 x})}{1 / (1 + e^{\beta_0 + \beta_1 x})} \right) = \log(e^{\beta_0 + \beta_1}) = \beta_0 + \beta_1 \\ logit(p(0)) &= \log(e^{\beta_0}) = \beta_0 \end{aligned} \right\} \text{linear in } x = 0, 1$$

$\psi := \frac{p(1)/(1-p(1))}{p(0)/(1-p(0))}$ “odds ratio”

$p(1) \approx 0, p(0) \approx 0 \Rightarrow \psi \approx \frac{p(1)}{p(0)}$ – relative risk

Odds ratio as dependency measure

Data

Y	X	
	0	1
0	a	b
1	c	d

Conditional distribution

Y	X	
	0	1
0	$1 - p(0)$	$1 - p(1)$
1	$p(0)$	$p(1)$

$p(j) = P(Y = 1|X = j) \quad j = 0, 1$ conditional distribution.

Want to see how $p(j)$ is changing.

$\psi = \frac{p(1)/(1-p(1))}{p(0)/(1-p(0))}$ measures change in conditional distributions.

$\psi = 1 \Leftrightarrow Y$ and X are independent

Unstructured model

$$\hat{p}^{obs}(\mathbf{x}) := \frac{\text{number of obs. with } Y = 1 \text{ and } \mathbf{X} = \mathbf{x}}{\text{number of obs. with } \mathbf{X} = \mathbf{x}} \quad x = 0, 1$$

$$\hat{p}^{obs}(1) = \frac{d}{b+d} \quad \hat{p}^{obs}(0) = \frac{c}{a+c} \Rightarrow \hat{\psi}^{obs} = \frac{\hat{p}^{obs}(1)/(1-\hat{p}^{obs}(1))}{\hat{p}^{obs}(0)/(1-\hat{p}^{obs}(0))} = \frac{da}{bc}$$

$$\Rightarrow \widehat{\log(\psi)}^{obs} = \log(\hat{\psi}^{obs}) \quad (\text{est. log odds ratio})$$

$$\widehat{Var}(\widehat{\log(\psi)}^{obs}) \approx \left(\frac{1}{a} + \frac{1}{b} + \frac{1}{c} + \frac{1}{d} \right) \quad (\text{est. var. of } \widehat{\log(\psi)}^{obs})$$

$$100(1 - \alpha)\% CI \text{ for } \log \psi : \quad \log \hat{\psi}^{obs} \pm z_{\alpha/2} \sqrt{\widehat{Var}(\log(\hat{\psi}^{obs}))}$$

$$100(1 - \alpha)\% CI \text{ for } \psi : \quad (e^{\log \hat{\psi}^{obs} - z_{\alpha/2} \sqrt{\widehat{Var}(\log(\hat{\psi}^{obs}))}}, e^{\log \hat{\psi}^{obs} + z_{\alpha/2} \sqrt{\widehat{Var}(\log(\hat{\psi}^{obs}))}})$$

Example: Survival on the Titanic

$$Y = \begin{cases} 1 & \text{survived} \\ 0 & \text{not survived} \end{cases}$$

$$X = \begin{cases} 1 & \text{male} \\ 0 & \text{female} \end{cases}$$

	X	
	0	1
0	154	709
1	308	142

$$\hat{p}(0) = \frac{308}{154+308} = 0.67$$

67% of females have survived

$$\hat{p}(1) = \frac{142}{709+142} = 0.17$$

17% of males have survived

$$\hat{o}(0) = \frac{\hat{p}(0)}{1-\hat{p}(0)} = \frac{0.67}{1-0.67} = 2$$

Women survived twice as often as not to survive

$$\hat{o}(1) = \frac{\hat{p}(1)}{1-\hat{p}(1)} = 0.2 = \frac{1}{5}$$

Men did not survive 5 times as often as to survive

$$\Rightarrow \hat{\psi} = \frac{\hat{o}(1)}{\hat{o}(0)} = \frac{0.2}{2} = 0.1 = \frac{1}{10}$$

Women had 10 times higher odds to survive compared to men

Polytomous covariate

Y	Category of X		
	1	\dots	J
0	$1 - p(1)$	\dots	$1 - p(J)$
1	$p(1)$	\dots	$p(J)$

Nominal categories

(Example: car marks: BMW, VW, Ford: *unordered*)

Model: $p(j) := P(Y = 1 | X = j) = \frac{e^{\beta_0 + \beta_1 I_1(i) + \dots + \beta_{J-1} I_{J-1}(i)}}{1 + e^{\beta_0 + \beta_1 I_1(i) + \dots + \beta_{J-1} I_{J-1}(i)}}$

$$I_j(i) = \begin{cases} 1 & x_i = j \\ 0 & \text{otherwise} \end{cases} \quad j = 1, \dots, J-1 \quad \textcolor{red}{\text{dummy coding}}$$

$$\Rightarrow p(J) = \frac{e^{\beta_0}}{1 + e^{\beta_0}} \quad \rightarrow \quad \beta_0 \quad \text{parametrizes} \quad \textcolor{red}{\text{logit}}(p(J))$$

Only $J - 1$ dummy variables are used to avoid a non full rank design matrix.

$$\Rightarrow \psi_j := \frac{p(j)/(1 - p(j))}{p(J)/(1 - p(J))} = e^{\beta_j} \quad \forall j = 1, \dots, J-1$$

J is *reference category*.

If $\psi_1 = \dots = \psi_{J-1}$: *constant odds ratio*

Example: Survival on the Titanic

Consider Pclass as nominal covariate

Y	Pclass		
	1	2	3
0	129	161	573
1	193	119	138
$\hat{p}^{obs}(j)$	$\frac{193}{129+193} = 0.60$	0.42	0.19
$\hat{o}^{obs}(j)$	$\frac{0.6}{1-0.6} = 1.50$	0.72	0.23
$logit(\hat{p}^{obs}(j))$	0.41	-0.33	-1.50
$\hat{\psi}^{obs}(j)$	$\frac{1.5}{0.23} = 6.50$	3.10	

First (second) class passengers had a 6.5 (3.1) times higher odds to survive compared to third class passengers → dependence between class and survival status

Ordinal categories

Examples: marks: A, B, C, D, E ; age groups.

Ordinal categories result often from **grouping** quantitative data.

Two coding possible:

-use **dummy** variables as with nominal categories

-use **scores**

Example:	Age groups			
	20 – 34	35 – 44	45 – 54	55 – 64
$s(j)$ scores (means)	27	39.5	49.5	59.5

$$p(j) = P(Y = 1 | X = j) = \frac{e^{\beta_0 + \beta_1 s(j)}}{1 + e^{\beta_0 + \beta_1 s(j)}} \Rightarrow \log\left(\frac{p(j)}{1 - p(j)}\right) = \beta_0 + \beta_1 s(j)$$

If there is **no functional** relationship between j and $\hat{p}^{obs}(j)$ (or $\log\left(\frac{\hat{p}^{obs}(j)}{1 - \hat{p}^{obs}(j)}\right)$) then a **dummy coding** is more appropriate.

Quantitative covariates

Binomial model: $Y_i|X_i = x_i \sim bin(n_i, p(x_i))$ independent

For a logistic model we have

$$logit(p(x_i)) = \beta_0 + \beta_1 x_i$$

This model is appropriate if $logit(\hat{p}^{obs}(x_i))$ linear in x .

Problem:

If $Y_i = 0$ or $Y_i = n_i$ we have

$$\log\left(\frac{\hat{p}^{obs}(x_i)}{1-\hat{p}^{obs}(x_i)}\right) = \log\left(\frac{Y_i/n_i}{1-Y_i/n_i}\right) = \log\left(\frac{Y_i}{n_i-Y_i}\right) \text{ undefined}$$

Consider therefore

$$\text{empirical logits: } l_{x_i} := \log\left(\frac{Y_i+1/2}{n_i-Y_i+1/2}\right)$$

Bernoulli model: $Y_i|X_i = x_i \sim \text{bern}(p(x_i))$ independent

$$\Rightarrow l_{x_i} = \begin{cases} \log\left(\frac{3/2}{1/2}\right) = \log(3) \approx 1.1 \\ \log\left(\frac{1/2}{3/2}\right) = \log(1/3) \approx -1.1 \end{cases}$$

Need smoothing to interpret the plot of x_i versus l_{x_i}

Other approach: group data to achieve an binomial response with an ordinal covariate. Proceed as before.

Titanic EDA for each covariate

The Splus function `main1.plot()` calculates **empirical logits** and plots them together with pointwise 95% Confidence limits.

```
> titanic.main      # Splus code
function(ps = F)
{
  Age.cut <- cut(Age, breaks = quantile(Age, probs =
                                         c(0, 0.2, 0.4, 0.6, 0.8, 1), na.rm = T))
  if(ps == T) {
    ps.options(colors = ps.colors.rgb[c("black", "cyan",
                                         "magenta", "green", "MediumBlue", "red"), ],
                horizontal = F)
    postscript(file = "titanic.main.ps")
  }
  par(mfrow = c(2, 2))
  main1.plot(Survived, Sex, "Sex")
  main1.plot(Survived, PClass, "PClass")
  main1.plot(Survived, Age.cut, "Age")
}
```

```
> titanic.main()
```

Main Effects for Sex

	female	male
emp. logit	0.69	-1.61
n	462.00	851.00

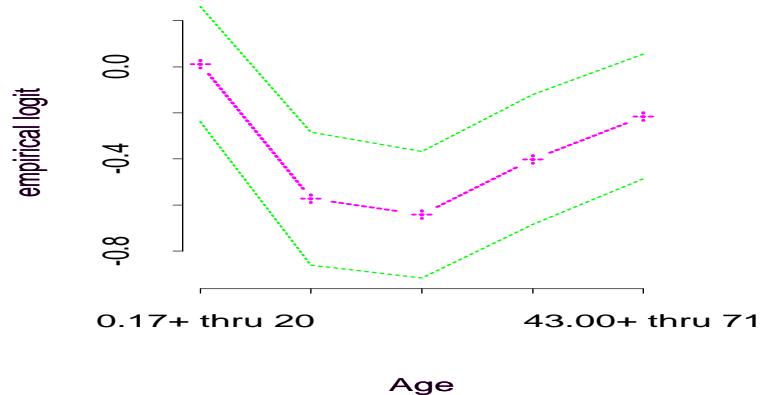
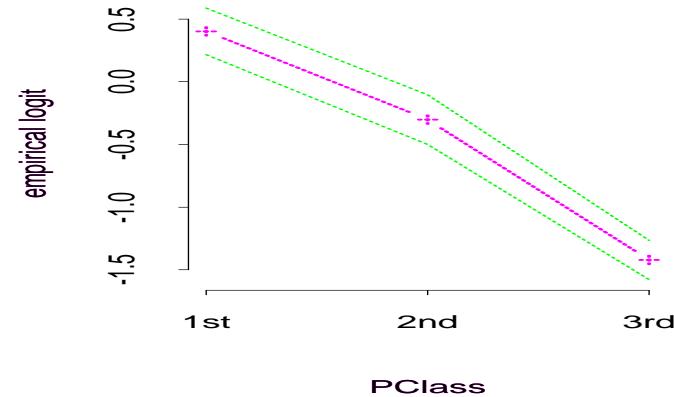
Main Effects for PClass

	1st	2nd	3rd
emp. logit	0.4	-0.3	-1.42
n	322.0	280.0	711.00

Main Effects for Age

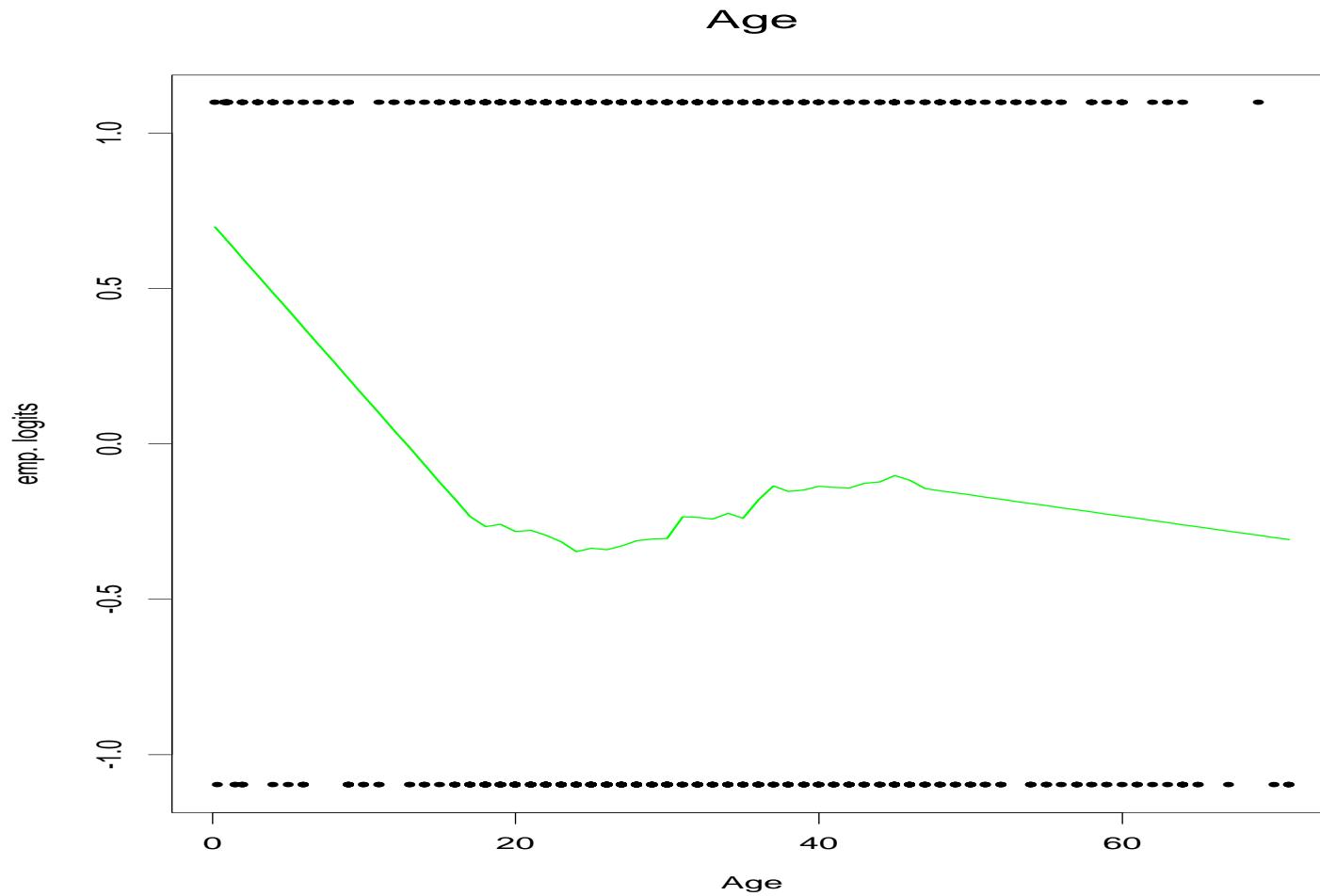
	0.17+ thru 20	20.00+ thru 25	25.00+ thru 32
emp. logit	0.01	-0.57	-0.64
n	171.00	139.00	157.00
	32.00+ thru 43	43.00+ thru 71	
emp. logit	-0.4	-0.22	
n	140.0	148.00	

For quantitative covariates a grouped variable using quintiles are used.



Quadratic Effect of Age?

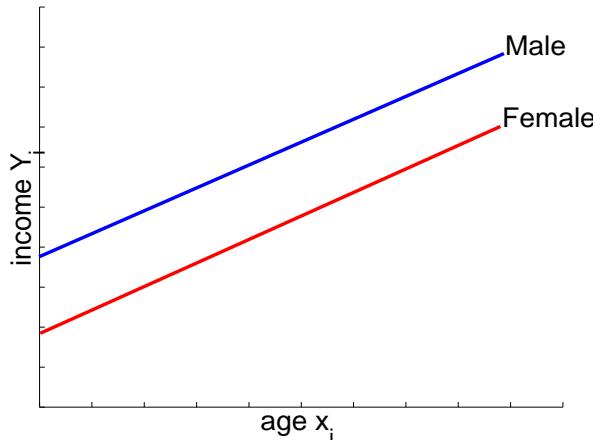
Smoothed empirical logits for binary Responses:



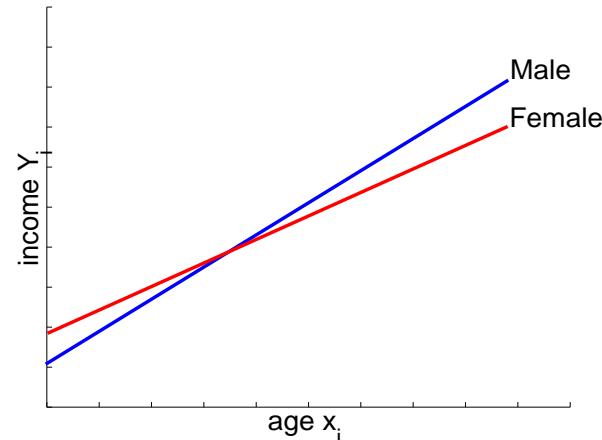
Indicates **nonlinear Age Effect**, but maybe not **quadratic**

Influence on $p(x)$ of several covariates

Linear models: one quantitative/one dichotomous



No interaction: difference in income independent of age
same slopes, different intercepts



Interaction: difference in income dependent of age
different slopes + intercepts

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 D_i + \beta_3 x_i \cdot D_i + \epsilon_i \quad D_i = \begin{cases} 1 & \text{male} \\ 0 & \text{female} \end{cases}$$

$$\begin{aligned} i \text{ male: } Y_i &= \beta_0 + \beta_1 x_i + \beta_2 + \beta_3 x_i + \epsilon_i = (\beta_0 + \beta_2) + (\beta_1 + \beta_3)x_i + \epsilon_i \\ i \text{ female: } Y_i &= \beta_0 + \beta_1 x_i + \epsilon_i \end{aligned}$$

Testing for interaction: $H_0 : \beta_3 = 0$ $H_1 : \beta_3 \neq 0$

If second covariate is polytomous with J levels use

$$D_{1i} = \begin{cases} 1 & \text{obs. } i \text{ has category 1} \\ 0 & \text{otherwise} \end{cases}$$
$$\vdots$$
$$D_{(J-1)i} = \begin{cases} 1 & \text{obs. } i \text{ has category } J-1 \\ 0 & \text{otherwise} \end{cases}$$

For interactions add terms $x_i D_{1i}, \dots, x_i D_{(k-1)i}$. Note category J is the reference category here.

If second covariate is quantitative use

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i1} \cdot x_{i2} + \epsilon_i$$

to model interaction.

Discovering interactions in logistic regression:

- Since the **logits** should be **linear** in the covariates one can look for **non parallel lines** when **empirical logits** are used.
- Confidence bands should be considered, when assessing **non parallelity**.

EDA of interaction effects for the Titanic data

```
> titanic.inter()
```

```
Interaction Effects for  Sex and PClass  
Empirical Logit
```

	PClass.1st	PClass.2nd	PClass.3rd
Sex.female	2.65	1.95	-0.50
Sex.male	-0.71	-1.76	-2.02

Cell Sizes

	PClass.1st	PClass.2nd	PClass.3rd
Sex.female	143	107	212
Sex.male	179	173	499

Interaction Effects for Sex and Age

Empirical Logit

	Age. 0.17+ thru 20	Age.20.00+ thru 25
Sex.female	0.80	0.77
Sex.male	-0.68	-1.56
	Age.25.00+ thru 32	Age.32.00+ thru 43
Sex.female	0.81	1.50
Sex.male	-1.38	-1.65
	Age.43.00+ thru 71	
Sex.female	1.93	
Sex.male	-1.58	

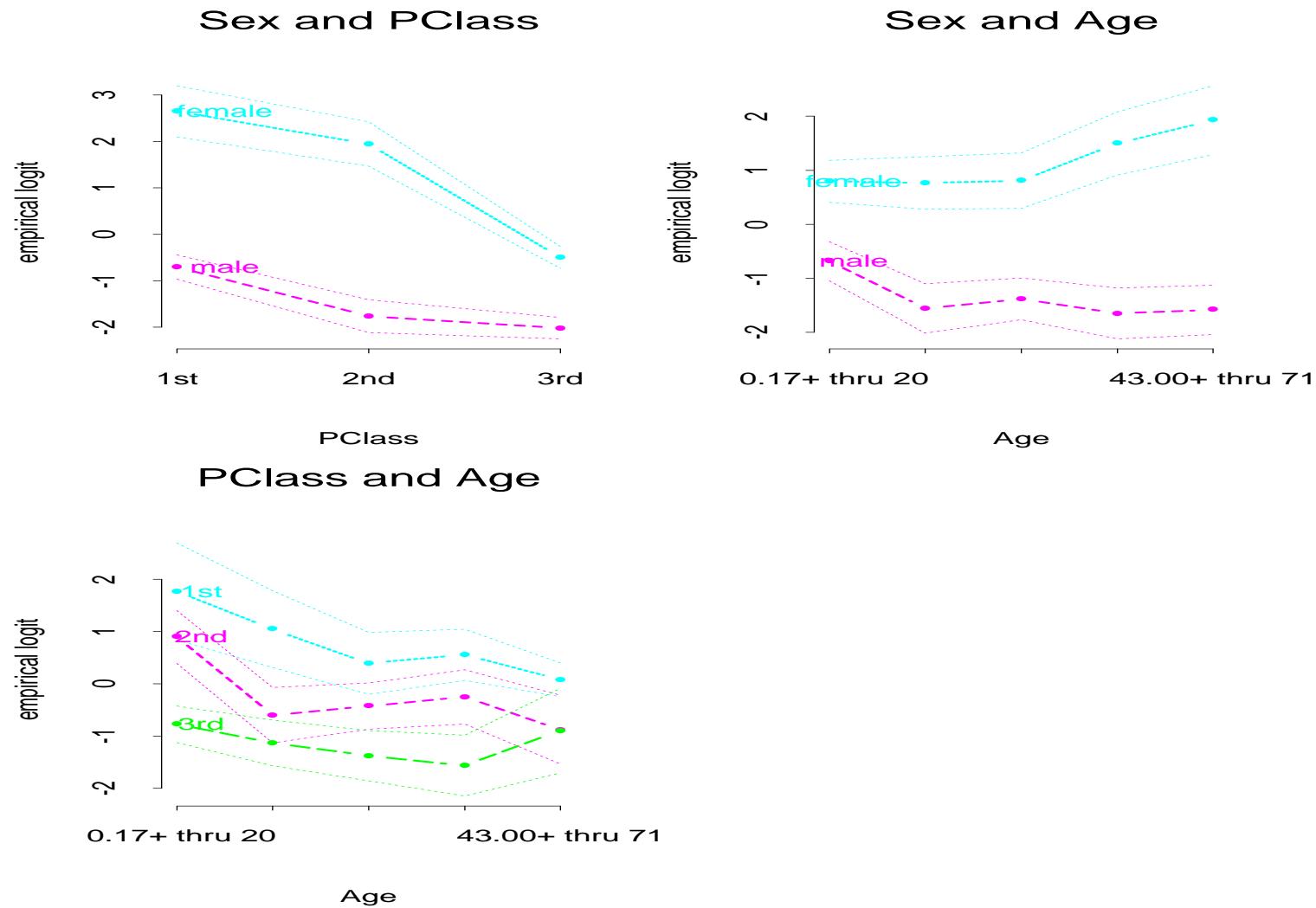
Cell Sizes

	Age. 0.17+ thru 20	Age.20.00+ thru 25
Sex.female	81	51
Sex.male	90	88
	Age.25.00+ thru 32	Age.32.00+ thru 43
Sex.female	46	51
Sex.male	111	89
	Age.43.00+ thru 71	
Sex.female	58	
Sex.male	90	

Interaction Effects for PClass and Age

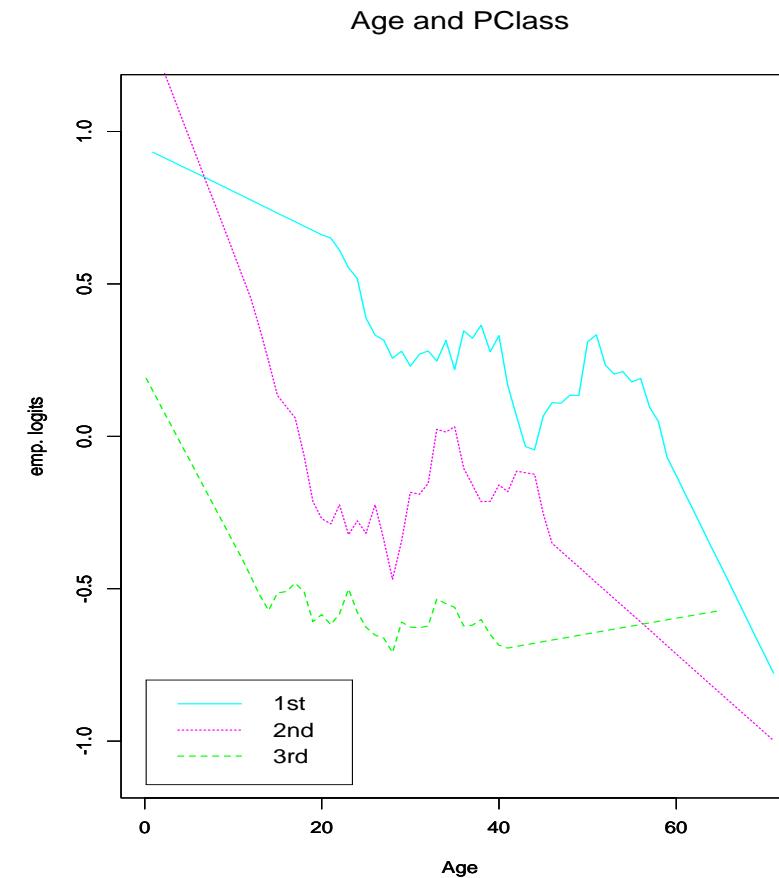
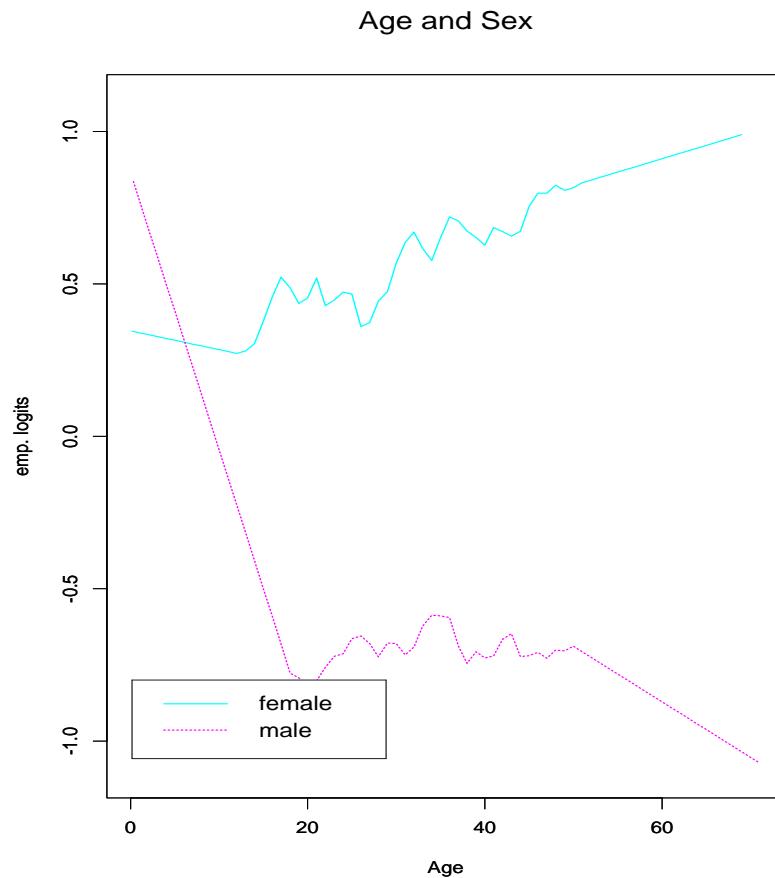
Empirical Logit

	Age. 0.17+ thru 20	Age.20.00+ thru 25
PClass.1st	1.77	1.05
PClass.2nd	0.90	-0.60
PClass.3rd	-0.78	-1.13
	Age.25.00+ thru 32	Age.32.00+ thru 43
PClass.1st	0.39	0.56
PClass.2nd	-0.43	-0.25
PClass.3rd	-1.38	-1.57
	Age.43.00+ thru 71	
PClass.1st	0.08	
PClass.2nd	-0.88	
PClass.3rd	-0.90	



Interaction Effects are present since lines are nonparallel

Smoothed Logits for Binary Responses:



Final notes to EDA in logistic regression

- EDA is only a screening methods. Hypotheses generated by the EDA have to be verified with **partial deviance** tests.
- **Binomial** models are needed to assess the fit with a **residual deviance** test.

References

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