Logistic Regression

Ariel Alonso Abad

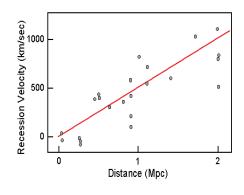
Catholic University of Leuven

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Linear regression

Basic model: $Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$

Hubble's Data (1929)

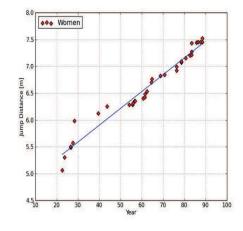


Hubble's law

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Linear regression

Basic model:
$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$$

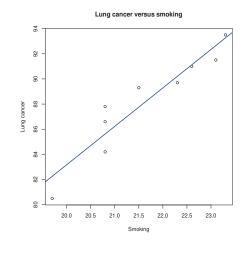


- Hubble's law
- Sport

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Linear regression

Basic model: $Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$

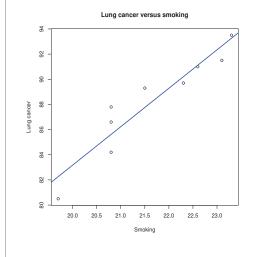


- Hubble's law
- Sport
- Smoking and lung cancer

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Linear regression

Basic model:
$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$$



- Hubble's law
- Sport
- Smoking and lung cancer
- Linear regression versus Logistic regression

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Legends of America: Donner party data

Donner party expedition

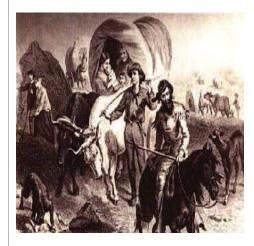
In 1846, the Donner and Reed families left Illinois for California, a 2500 mile journey that would become one of the greatest tragedies in USA history. Stranded in Sierra Nevada by a series of snowstorms, they were rescued in April of the following year. 40 members died, some (or perhaps all) of those that survived did so by resorting to cannibalism.

TRAIL OF THE DONNER PARTY



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Donner party data



- 88 persons
- Variables: survival, gender and age
- Taking into account age, are the chances of survival larger for women than for men?

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Donner party data

Name	Sex	Age	Surviva
Antoine	Male	23	No
Breen, Mary	Female	40	Yes
Breen, Patrick	Male	40	Yes
Burger, Charles	Male	30	No
Denton, John	Male	28	No
Dolan, Patrick	Male	40	No
Donner, Elizabeth	Female	45	No
Donner, George	Male	62	No
Donner, Jacob	Male	65	No
Donner: Tamsen	Female	45	No
Eddy, Eleanor Eddy, William	Female	25	No
Eddy, William	Male	28	Yes
Elliot, Milton	Male	28	No
Fosdick, Jay	Male	23	No
Fosdick, Sarah	Female	22	Yes
Foster, Sarah	Female	23	Yes
Foster, William	Male	28	Yes
Graves, Eleanor	Female	62 65 45 25 28 23 223 223 28 15 47	Yes
Graves, Elizabeth	Female	47	No
Graves, Franklin	Male	5.7	No
Graves, Franklin Graves, Mary	Female	57 20 18	Yes
Graves, William	Male	18	Yes
Halloran, Luke	Male	25 60	No
Hardkoop, Mr. Herron, William	Male	.60	No
Herron, William	Male	25	Yes
Noah, James	Male	20	Yes
Keseberg, Lewis	Male Male Female Female Male	20 32 32 24 30	Yes
Keseberg, Phillipine	Female	32	Yes
Keseberg, Phillipine McCutcheon, Amanda	Female	24	Yes
McCutcheon, William	Male	30	Yes
Murphy, John	Male	15	No
Murphy, Lavina	Female	50	No
Pike, Harriet	Female	21	Yes
Pike, William	Male	25	No
Reed, James	Male	46	Yes
Reed, Margaret	Female	32	Yes
Reinhardt, Joseph	Male	30	No
Shoemaker, Samuel	Male	25	No
Smith, James	Male	25	No
Snyder, John	Male	25	No
Spitzer, Augustus	Male	30	No
Stanton, Charles	Male	320 255 255 255 30 355	No
Trubode, J.B.	Male	2.5	Yes
Williams, Baylis	Male	23 24 25	No
Williams, Eliza	Female	25	Yes

• Dependent variable is binary:

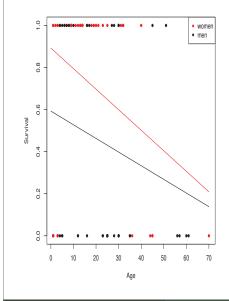
$$Y = \begin{cases} 1 \text{ Survived,} \\ 0 \text{ Died.} \end{cases}$$

Independent predictors:

$$age, fem = \begin{cases} 1 \text{ for women,} \\ 0 \text{ for men.} \end{cases}$$

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Exploring the data



- Survived = 1, Died = 0
- Graph is not as informative as in linear regression

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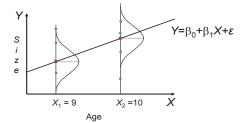
Linear regression

- Basic model: $Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$
- The expected value (average) of Y is modeled as a linear function of the predictors

$$E(Y|X_1,X_2,\ldots,X_p) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

Simple linear regression

Size versus age



 $Y = \beta_0 + \beta_1 X + \varepsilon$

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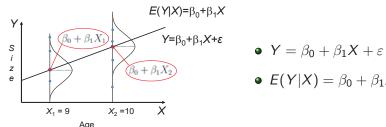
Linear regression

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$$E(Y|X_1,X_2,\ldots,X_p) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

Simple linear regression

Size versus age



- $\bullet \ E(Y|X) = \beta_0 + \beta_1 X$

Binary outcome: Problem

The expected value (average) of a binary variable is a probability

$$E(Y|X_1, X_2, ..., X_p) = P(Y = 1|X)$$

where P(Y=1|X) gives the probability as a function of the covariates $\boldsymbol{X} = (X_1, X_2, \dots, X_p)$

$$P(Y = 1|\mathbf{X}) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

$$0 \le P(Y = 1|\mathbf{X}) \le 1$$

but $\eta(\mathbf{X}) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$ is not always between 0 and 1.

Binary outcome: Problem

The expected value (average) of a binary variable is a probability

$$E(Y|X_1, X_2, ..., X_p) = P(Y = 1|X)$$

where $P(Y=1|\pmb{X})$ gives the probability as a function of the covariates $\pmb{X}=(X_1,X_2,\ldots,X_p)$

$$P(Y=1|age, fem) = eta_0 + eta_1 age + eta_2 fem$$
 $0 \leq P(Y=1|age, fem) \leq 1$

but $\eta(age, fem) = \beta_0 + \beta_1 age + \beta_2 fem$ is not always between 0 and 1.

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Binary outcome: Problem

Problem with the linear model

$$P(Y = 1 | fem) = \beta_0 + \beta_1 fem$$

Assume that $\beta_0=0.5$ en $\beta_1=-1$. What is the survival probability for a woman?

$$P(Y = 1 | fem) = 0.5 - fem$$

For women: fem = 1 thus

$$P(Y = 1|fem = 1) = 0.5 - fem$$

= $0.5 - 1 = -0.5$

A probability should always be between 0 and 1!

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Binary outcome: Solution

• Transform P(Y = 1 | X):

$$\operatorname{logit}\left[P(Y=1|\boldsymbol{X})\right] = \operatorname{ln}\frac{P(Y=1|\boldsymbol{X})}{P(Y=0|\boldsymbol{X})} = \operatorname{ln}\left(\frac{P(Y=1|\boldsymbol{X})}{1 - P(Y=1|\boldsymbol{X})}\right)$$

- $-\infty \leq \text{logit}[P(Y=1|X)] \leq \infty$
- Model:

$$logit [P(Y=1|X)] = \eta(X) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

• Transform back:

$$P(Y=1|X) = \frac{e^{\eta(X)}}{1+e^{\eta(X)}}$$

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Binary outcome: Solution

• Transform P(Y = 1 | X):

$$\operatorname{logit}\left[P(Y=1|\boldsymbol{X})\right] = \operatorname{ln}\frac{P(Y=1|\boldsymbol{X})}{P(Y=0|\boldsymbol{X})} = \operatorname{ln}\left(\frac{P(Y=1|\boldsymbol{X})}{1 - P(Y=1|\boldsymbol{X})}\right)$$

- $-\infty \leq \text{logit}[P(Y=1|X)] \leq \infty$
- Model:

logit
$$[P(Y = 1|X)] = \eta(X) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

• Transform back:

$$P(Y=1|\boldsymbol{X}) = \frac{e^{\eta(\boldsymbol{X})}}{1+e^{\eta(\boldsymbol{X})}} = \frac{e^{\beta_0+\beta_1X_1+\cdots+\beta_pX_p}}{1+e^{\beta_0+\beta_1X_1+\cdots+\beta_pX_p}}$$

• Now is P(Y = 1 | X) always between 0 en 1

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Binary outcome: Solution

• Transform P(Y = 1 | X):

$$\operatorname{logit}\left[P(Y=1|\boldsymbol{X})\right] = \operatorname{ln}\frac{P(Y=1|\boldsymbol{X})}{P(Y=0|\boldsymbol{X})} = \operatorname{ln}\left(\frac{P(Y=1|\boldsymbol{X})}{1 - P(Y=1|\boldsymbol{X})}\right)$$

- $-\infty \leq \text{logit}[P(Y=1|X)] \leq \infty$
- Model:

$$logit[P(Y = 1|age, fem)] = \eta(age, fem) = \beta_0 + \beta_1 age + \beta_2 fem$$

• Transform back:

$$P(Y=1|\textit{age},\textit{fem}) = \frac{e^{\eta(\textit{age},\textit{fem})}}{1+e^{\eta(\textit{age},\textit{fem})}} = \frac{e^{\beta_0+\beta_1\textit{age}+\beta_2\textit{fem}}}{1+e^{\beta_0+\beta_1\textit{age}+\beta_2\textit{fem}}}$$

• Now is P(Y = 1 | age, fem) always between 0 en 1

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Binary outcome: Solution

Logistic Model

$$P(Y=1|\mathit{fem}) = rac{e^{eta_0 + eta_1 \mathit{fem}}}{1 + e^{eta_0 + eta_1 \mathit{fem}}}$$

Assume that $\beta_0=0.5,\ \beta_1=-1.$ What is the survival probability for a woman?

$$P(Y = 1|fem) = \frac{e^{0.5 - fem}}{1 + e^{0.5 - fem}}$$

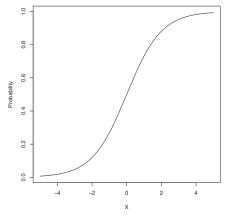
For women: fem = 1 thus

$$P(Y = 1 | fem = 1) = \frac{e^{0.5-1}}{1 + e^{0.5-1}} = \frac{e^{-0.5}}{1 + e^{-0.5}} = 0.378$$

Now the survival probability for a woman is between 0 en 1!

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Model for the probability: X continuous



$$P(Y=1|X) = \frac{e^X}{1+e^X}$$

Logarithm (log)

Different notations: log

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Estimating the parameters

logit
$$[P(Y = 1|X)] = \eta(X) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p$$

- Ordinary least squares (OLS) is not suitable
- Method of maximum likelihood (ML) is the adequate choice

Maximum Likelihood Estimation

Find the values of the parameters so that the likelihood is maximized. In other words, the ML estimates (MLE) are the values of the parameters that make the observed data most likely to have been observed. For linear models OLS and ML are equivalent.

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Fitting the model in R

Fitting the model in R

Logistic Regression

Fitting the model in R

Donner party data

Model

logit
$$[P(Y = 1 | age, fem)] = \beta_0 + \beta_1 age + \beta_2 fem$$

where fem = 1 for women fem = 0 for men. Equivalently

$$P(Y=1|age, fem) = rac{e^{eta_0 + eta_1 age + eta_2 fem}}{1 + e^{eta_0 + eta_1 age + eta_2 fem}}$$

Estimated model

logit
$$\left[\hat{P}(Y=1|age, fem)\right] = 0.553 - 0.035age + 1.067fem$$

$$\hat{P}(Y=1|age,fem) = \frac{e^{0.553-0.035age+1.067fem}}{1+e^{0.553-0.035age+1.067fem}}$$

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Interpretation of the coefficients

Linear regression model

$$Y = \beta_0 + \beta_1 X + \varepsilon$$

- Association between (y,x): $r_{xy} = \frac{\text{cov}(x,y)}{\sigma_y \sigma_x}$
 - Range: $-1 \le r_{xy} \le 1$
 - Positive correlation between x en y: $r_{xy} > 0$ $(\beta_1 > 0)$
 - No correlation between x en y: $r_{xy}=0$ ($\beta_1=0$)
 - \bullet Negative correlation between x en y: r_{xy} < 0 ($\beta_1 < 0)$
- $\bullet \ \beta_1 = \mathsf{r}_{\mathsf{x}\mathsf{y}} \frac{\sigma_{\mathsf{y}}}{\sigma_{\mathsf{x}}}$

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Association in a 2×2 cross-table

Hypothetical example

Predictor

		Female $\mathit{fem} = 1$	Male $fem = 0$
riterium	Survived $(Y = 1)$	$P(Y=1)=\frac{2}{3}$	$P(Y=1)=\frac{1}{3}$
Crite	Died $(Y = 0)$	$P(Y=0)=\frac{1}{3}$	$P(Y=0)=\tfrac{2}{3}$

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Association in a 2×2 cross-table

Odds

• Odds of surviving for women:

$$\Theta_{\textit{survival}|\textit{women}} = \frac{P(\textit{Y} = 1|\textit{fem} = 1)}{P(\textit{Y} = 0|\textit{fem} = 1)} = \frac{2/3}{1/3} = 2$$

- \Rightarrow for every 2 women that survive 1 dies
- Odds of surviving for men:

$$\Theta_{survival|men} = \frac{P(Y=1|fem=0)}{P(Y=0|fem=0)} = \frac{1/3}{2/3} = \frac{1}{2} = 0.5$$

 \Rightarrow for every man that survives 2 die

(term comes from horse racing)

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Association in a 2×2 cross-table

Odds Ratio

Ratio of odds or odds ratio = is a measure of association in 2×2 cross-tables

Odds Ratio:
$$OR = \frac{\Theta_{survival|women}}{\Theta_{survival|men}} = \frac{2}{0.5} = 4$$

• Interpretation: the odds of survival for women are 4 times larger than the odds of survival for men

(if the odds for men are 0.5 to 1 then for women they are 2 to 1)

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Association in a 2×2 cross-table

Predictor

		X = 1	X = 0
		Female	Male
ium	Y = 1	$P(Y=1)=\tfrac{2}{3}$	$P(Y=1)=\tfrac{2}{3}$
riterium	Y = 0	$P(Y=1)=\frac{1}{3}$	$P(Y=1)=\frac{1}{3}$
\cup			

$$\Theta_{survival|women} = \frac{P(Y=1|fem=1)}{P(Y=0|fem=1)} = \frac{2/3}{1/3} = 2$$

$$\Theta_{survival|men} = \frac{P(Y = 1|fem = 0)}{P(Y = 0|fem = 0)} = \frac{2/3}{1/3} = 2$$

$$OR = \frac{\Theta_{survival|women}}{\Theta_{survival|men}} = \frac{2}{2} = 1$$

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Properties of odds ratios

Odds Ratio

- $0 < OR < \infty$
- ullet $OR = 1 \Leftrightarrow \text{independence}$
- ullet $OR > 1 \Leftrightarrow$ positive association
- $OR < 1 \Leftrightarrow$ negative association

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Interpretation of the coefficients

Dichotomous predictor (X=0 of 1 like gender) probability model

$$P(Y=1|X) = rac{e^{eta_0 + eta_1 X}}{1 + e^{eta_0 + eta_1 X}} = \left\{ egin{array}{c} rac{e^{eta_0 + eta_1}}{1 + e^{eta_0 + eta_1}} & X=1, ext{female} \ \ rac{e^{eta_0}}{1 + e^{eta_0}} & X=0, ext{male} \end{array}
ight.$$

Predictor

	X = 1		X = 0	
		Female	Male	
Criterium	Y=1 Survived	$P(Y = 1) = \frac{e^{\beta_0 + \beta_1}}{1 + e^{\beta_0 + \beta_1}}$	$P(Y=1) = \frac{e^{\beta_0}}{1 + e^{\beta_0}}$	
	Y = 0 Died	$P(Y = 0) = \frac{1}{1 + e^{\beta_0 + \beta_1}}$	$P(Y=0)=\frac{1}{1+e^{\beta_0}}$	

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Computing the odds ratio

Predictor

$$OR = \frac{P(Y = 1|X = 1)/P(Y = 0|X = 1)}{P(Y = 1|X = 0)/P(Y = 0|X = 0)}$$

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Computing the odds ratio

Predictor

		X = 1	X = 0
		Female	Male
u	V 1	$e^{eta_0+eta_1}$	e^{eta_0}
riterium	Y = 1	$1 + e^{\beta_0 + \beta_1}$	$\overline{1+e^{eta_0}}$
rite	Y = 0	1	1
Ċ	I = 0	$1+e^{eta_0+eta_1}$	$\overline{1+e^{eta_0}}$

$$OR = rac{rac{e^{eta_0 + eta_1}}{1 + e^{eta_0 + eta_1}} igg/rac{1}{1 + e^{eta_0 + eta_1}}}{rac{e^{eta_0}}{1 + e^{eta_0}} igg/rac{1}{1 + e^{eta_0}}} = e^{eta_1}$$

$$OR = e^{\beta_1}$$

$$In(OR) = \beta_1$$

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Donner party data

- $logit(\hat{P}(Y = 1|age, fem)) = 0.553 0.035age + 1.067fem$
- Gender: The odds of survival for a woman are 3 times larger than the odds of survival for a man of the same age: $\hat{OR}=e^{1.067}\approx 3$





$$\Theta_{\textit{survival}|\textit{women}} = 3 \cdot \Theta_{\textit{survival}|\textit{men}}$$

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Donner party data

- $logit(\hat{P}(Y = 1|age, fem)) = 0.553 0.035age + 1.067fem$
- Gender: The odds of survival for a woman are 3 times larger than the odds of survival for a man of the same age: $\hat{OR} = e^{1.067} \approx 3$





$$\Theta_{survival|women} = 3 \cdot \Theta_{survival|men}$$

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Interpretation of the coefficients

Logistic regression model

logit
$$[P(Y = 1|X)] = \beta_0 + \beta_1 X$$

- Association between (y, x): OR
 - ullet Range: $0 < OR < \infty$
 - Positive association between x en y: OR > 1 $(\beta_1 > 0)$
 - No association between x en y: $\mathit{OR}=1$ $(\beta_1=0)$
 - Negative association between x en y: $OR < 1 \ (\beta_1 < 0)$
- $\beta_1 = \ln(OR)$

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Continuous predictor X

- The interpretation is analogous to the one given for dummy predictor
- For instance, consider two ages
 - A1: Age=*X*
 - A2: A year older, Age=X + 1

$$\Theta_{\textit{survival}|X+1} = \frac{P(Y=1|X+1)}{P(Y=0|X+1)} \qquad \Theta_{\textit{survival}|X} = \frac{P(Y=1|X)}{P(Y=0|X)}$$

$$\Theta_{\mathit{survival}|X+1} = e^{eta_1} \cdot \Theta_{\mathit{survival}|X}$$

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Donner party data

- $logit(\hat{P}(Y = 1|age, fem)) = 0.553 0.035age + 1.067fem$
- Age: $\hat{\beta}_1 = -0.0356 \Rightarrow \hat{OR} = e^{-0.0356} = 0.965 \approx 0.96$, an increase of one year in age is associated with a 4% decrease in the odds of survival





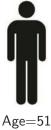
Age=25

$$\Theta_{survival|26,men} = 0.96 \cdot \Theta_{survival|25,men}$$

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Donner party data

- $logit(\hat{P}(Y = 1|age, fem)) = 0.553 0.035age + 1.067fem$
- ullet Age: $\hat{eta}_1 = -0.0356 \Rightarrow \hat{OR} = e^{-0.0356} = 0.965 pprox 0.96$, an increase of one year in age is associated with a 4% decrease in the odds of survival





$$\Theta_{\textit{survival}|51,\textit{men}} = 0.96 \cdot \Theta_{\textit{survival}|50,\textit{men}}$$

Logistic Regression

Continuous predictor X

- A one unit change in X is not always meaningful
- For instance, consider two ages
 - A1: Age=*X*
 - A2: c years older, Age=X + c

$$\Theta_{survival|X+c} = \frac{P(Y=1|X+c)}{P(Y=0|X+c)} \qquad \Theta_{survival|X} = \frac{P(Y=1|X)}{P(Y=0|X)}$$

$$\Theta_{survival|X} = \frac{P(Y=1|X)}{P(Y=0|X)}$$

$$\Theta_{survival|X+c} = e^{\beta_1 \cdot c} \cdot \Theta_{survival|X}$$

Donner party data

- $logit(\hat{P}(Y = 1|age, fem)) = 0.553 0.035age + 1.067fem$
- Age: $\hat{\beta}_1=-0.0356\Rightarrow\hat{OR}=e^{-0.0356\cdot 10}=0.70$, a 10 years increase in age is associated with a 30% decrease in the odds of survival





$$\Theta_{survival|30,women} = 0.70 \cdot \Theta_{survival|20,women}$$

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Donner party data

- $logit(\hat{P}(Y = 1|age, fem)) = 0.553 0.035age + 1.067fem$
- Age: $\hat{\beta}_1 = -0.0356 \Rightarrow \hat{OR} = e^{-0.0356 \cdot 10} = 0.70$, a 10 years increase in age is associated with a 30% decrease in the odds of survival





 $\Theta_{survival|60,women} = 0.70 \cdot \Theta_{survival|50,women}$

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More predictors

- ullet The same approach as above: change in logit cause by increasing predictor X_j by 1 unit and keeping all the other predictors fixed is back transformed into a change in odds ratio
- Often called "adjusted odds ratio" ("adjusted" by other predictors)

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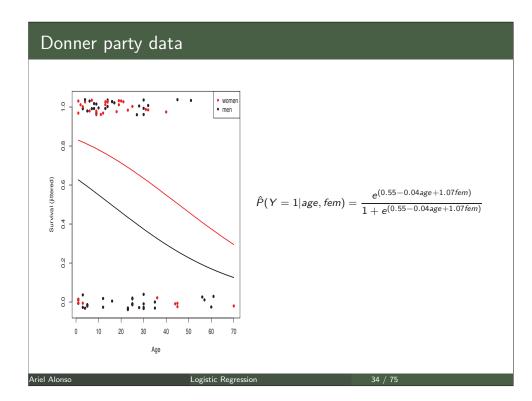
Donner party data

Estimated model

$$logit(\hat{P}(Y = 1|age, fem)) = 0.553 - 0.035age + 1.067fem$$

- Gender: The survival odds for a woman are 3 times larger than the survival odds for a man of the same age: $\hat{OR} = e^{1.067} \approx 3$
- Age: A 10 year increase in age is associated with a 30% decrease in the survival odds for both men and women ($\hat{OR} = e^{-0.0356 \cdot 10} = 0.70$)

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Donner party data: Model fit

Model fit

Parameter	Estimate	Std. Error	z value	p-value
(Intercept)	0.553	0.417	1.325	0.1850
Age	-0.035	0.015	-2.336	0.0195
fem	1.067	0.482	2.214	0.0268

 $\bullet~95\%$ confidence interval for effect: Age, β_1

$$\left[\hat{eta}_1 - 1.96 \cdot SE(\hat{eta}_1), \hat{eta}_1 + 1.96 \cdot SE(\hat{eta}_1)\right]$$

• 95% BI for β_1 : $-0.035 \pm 1.96 \cdot 0.015 \Rightarrow (-0.067, -0.006)$

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Donner party data: Model fit

Model fit

Parameter	Estimate	Std. Error	z value	p-value
(Intercept)	0.553	0.417	1.325	0.1850
Age	-0.035	0.015	-2.336	0.0195
fem	1.067	0.482	2.214	0.0268

ullet 95% confidence interval for odds ratio: Age, $\mathit{OR} = e^{\beta_1}$

$$\left[\exp\left(\hat{\beta}_1 - 1.96 \cdot \textit{SE}(\hat{\beta}_1)\right), \exp\left(\hat{\beta}_1 + 1.96 \cdot \textit{SE}(\hat{\beta}_1)\right)\right]$$

• 95% BI for $OR = e^{\beta_1}$: $(e^{-0.067}, e^{-0.006}) = (0.934, 0.993)$

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Estimating odds ratios in R

```
> ## Odds ratios
  > exp(donner.log$coefficients)
  (Intercept)
                   Age
    1.7398953 0.9650211 2.9094868 e^{\beta_0}, e^{\beta_1}, e^{\beta_2}
  > exp(confint(donner.log))
  Waiting for profiling to be done... 2.5 % 97.5 %
  (Intercept) 0.7748972 4.0431170
          0.9348223 0.9930661
              1.1543365 7.7529827
  > exp(cbind(OR =donner.log$coefficients, confint(donner.log)))
  Waiting for profiling to be done...
                    OR 2.5 % 97.5 %
  (Intercept) 1.7398953 0.7748972 4.0431170
             0.9650211 0.9348223 0.9930661
  fem
               2.9094868 1.1543365 7.7529827
Ariel Alonso
```

Estimating odds ratios in R

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Plotting the survival probabilities in R

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Predicting the outcome

- One can use the model to predict the outcome of certain groups of interest
- For instance, in the Donner party study one may want to predict
 - The survival probability of a man with an average age (20.22 years)
 - The survival probability of a woman with an average age (20.22 years)

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Predicting the outcome

Donner party example:

$$logit \left[\hat{P}(Y=1|age, fem)
ight] = 0.553 - 0.035age + 1.067fem$$

with fem = 1 for women and fem = 0 for men

a) Survival probability for a man with the average age 20.22 (fem = 0)

$$\hat{P}(Y = 1|20.22, man) = \frac{e^{(0.553 - 0.035 \cdot 20.22 + 1.067 \cdot 0)}}{1 + e^{(0.553 - 0.035 \cdot 20.22 + 1.067 \cdot 0)}} = \frac{e^{-0.1547}}{1 + e^{-0.1547}}$$

$$= \frac{0.8566}{1.8566} = 0.4614$$

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Predicting the outcome

Donner party example:

$$\mathsf{logit}\left[\hat{P}(\mathit{Y}=1|\mathit{age},\mathit{fem})
ight] = 0.553 - 0.035\mathit{age} + 1.067\mathit{fem}$$

with fem = 1 for women and fem = 0 for men

b) Survival probability for a woman with the average age 20.22 (fem = 1)

$$\hat{P}(Y = 1|20.22, woman) = \frac{e^{(0.553 - 0.035 \cdot 20.22 + 1.067)}}{1 + e^{(0.553 - 0.035 \cdot 20.22 + 1.067)}}$$
$$= \frac{e^{0.9123}}{1 + e^{0.9123}} = \frac{2.49}{3.49} = 0.7134$$

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Predicting the outcome in R

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Model building and model selection

Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful.

George E. P. Box

- Until now we have pretended that the relevant covariates and the structure of the model are both known
- In reality the situation is often more complex: frequently neither the relevant covariates nor the structure of the model are known before hand

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Model building and model selection

- Thus, in practice scientists often consider several models (theories) to describe and explain reality
- For instance, in the Donner party example one may wonder if the effect of gender on survival varies across age or not, i.e., one may want to consider the model

logit
$$\left[\hat{P}(Y=1|age, fem)\right] = \beta_0 + \beta_1 age + \beta_2 fem + \beta_3 age \cdot fem$$

= $\beta_0 + \beta_1 age + (\beta_2 + \beta_3 \cdot age) fem$

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Interaction model in R

Interaction model

$$\mathsf{logit}\left[\hat{P}(\mathsf{Y}=1|\mathsf{age}, \mathit{fem})\right] = 0.398 - 0.028 \mathit{age} + 1.478 \mathit{fem} - 0.020 \mathit{age} \cdot \mathit{fem}$$

For women fem = 1

logit
$$\left[\hat{P}(Y = 1 | age, women)\right] = 0.398 - 0.028age + 1.478 - 0.020age$$

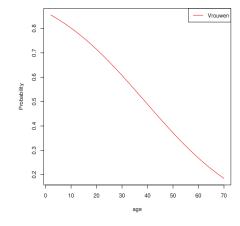
= 1.876 - 0.048age

$$\hat{P}(Y = 1 | age, women) = \frac{e^{1.876 - 0.048age}}{1 + e^{1.876 - 0.048age}}$$

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Interaction model

For women fem = 1



$$\hat{P}(Y=1|age) = \frac{e^{1.876-0.048age}}{1+e^{1.876-0.048age}}$$

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Interaction model

For men fem = 0

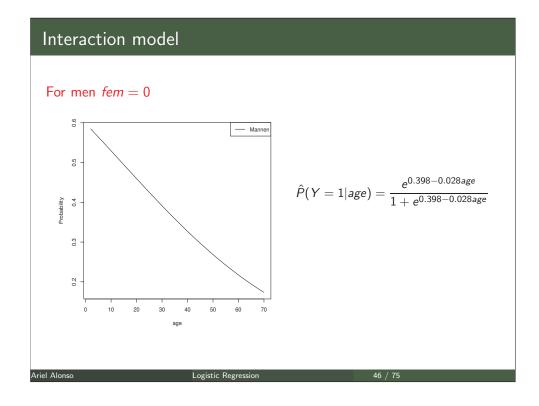
$$logit \left[\hat{P}(Y = 1 | age, men) \right] = 0.398 - 0.028age$$

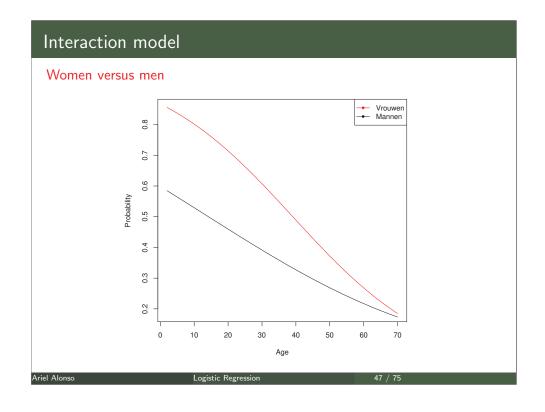
$$\hat{P}(Y=1|age,men) = \frac{e^{0.398-0.028age}}{1+e^{0.398-0.028age}}$$

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Donner party data

• How do the odds of survival of a woman compare to those of a 10 years younger woman?

ullet For women: logit $\Big[\hat{P}(Y=1|age,women)\Big]=1.876-0.048age$

• $OR(age + 10, age) = Exp(\hat{\beta}_1 \cdot 10) = e^{-0.48} = 0.62$





 $\Theta_{survival|30,women} = 0.62 \cdot \Theta_{survival|20,women}$

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Donner party data

- How do the odds of survival of a woman compare to those of a 10 years younger woman?
- ullet For women: logit $\Big[\hat{P}(Y=1|age,women)\Big]=1.876-0.048age$
- $OR(age + 10, age) = Exp(\hat{\beta}_1 \cdot 10) = e^{-0.48} = 0.62$





Age=50

 $\Theta_{survival|60,women} = 0.62 \cdot \Theta_{survival|50,women}$

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Donner party data

- How do the odds of survival of a woman compare to those of a 10 years younger woman?
- ullet For women: logit $\Big| \hat{P}(Y=1|age, women) \Big| = 1.876 0.048age$
- $OR(age + 10, age) = Exp(\hat{\beta}_1 \cdot 10) = e^{-0.48} = 0.62$

$$OR(age+10, age) = \frac{Odds(survival, age+10)}{Odds(survival, age)} = Exp(\hat{\beta}_1 \cdot 10) = e^{-0.48} = 0.62$$

Interpretation

A 10 years increase in age is associated with a 40% (30% in the model without interaction) decrease in the odds of survival

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Where do the models come from?

- Sometimes a set of models is provided based on subject-matter theory, the so-called mechanistic models. One example is the PK/PD models used in pharmacokinetic/pharmacodynamics
- In practice good theory is very rare. Most often some simple restrictions are placed on the behavior one expects to find, for example, linear models, factorial models with limited interactions, etc. These models are sometimes called empirical models
- Nowadays model classes are available that can approximate many data generating mechanism. Furthermore, the computational resources to fit such models are rapidly increasing
- Model building and model selection

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Model building: General principles

- Goal: To find a model that fits the data reasonably well without unnecessary complexity
- Model building is art and science: There are no clear, defined and fixed rules that you can automatically follow, but just general principles
- P1 Use your previous scientific knowledge
 - What are the research questions?
 - What does the theory say?
 - Are there results from previous studies?
 - What does the common sense suggest?

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Model building: General principles

- P2 Interactions between predictors in the model should be included based on theory and plausibility
 - Usually it is not necessary to evaluate all possible interactions
 - Interactions between more than two predictors: very sound theoretical considerations necessary to include them
- **P3** There is a preference for so-called *hierarchical models* (also known as the principle of marginality)
 - If the model includes an interaction, the corresponding main effects should be included as well
 - If the model includes a quadratic term (x^2) , a linear term should be included as well
 - An intercept should be always included

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Model building: General principles

- P4 There is a distinction between observational and experimental studies
 - Experimental research: Often limited set of factors is examined
 - Model construction often less important ("true" model may be almost completely determined by the design)
- **P5** Importance of **replication**: A single study is **not** conclusive evidence of existence of an effect
- **P6** Groups or sets of predictors may belong together and, hence, move together in and out of the model
 - For instance, personality can be represented using five predictors, the five factors of the Big Five
 - For instance, a categorical predictor with more than two categories is included in the model using a set of dummy variables. In the final model, these dummy variables may or may not be included together

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Model building: General principles

- P7 Be aware of the issues associated with automatic selection procedures (stepwise, forward, backward, etc.)
 - Each test is conditional on the results of the previous tests
 - Distribution of these conditional statistics not fully understood
 - \bullet Problems with the frequentist interpretation of α
 - Multiple comparison problem
 - In which sense is the final model best or optimal?
 - No measure of model uncertainty
- P8 Construction of a model is an iterative and creative process

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Model building: General principles

- P9 Inference after model construction and model selection: There is debate over which approach is correct. Active research area
- P10 The objective of a study may also be the prediction of the criterion
 - For instance, researchers may want to use a predictor(s) X to predict an outcome(s) Y
 - *Understanding* is less important and, therefore, other principles can play a role

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Explanation vs Prediction

- Explanation is like doing scientific research.
- Prediction is like doing engineering development. All that matters is that it works. And if the aim is prediction, model choice should be based on the quality of the predictions
- Why select a model at all?
 - It does seem a widespread misconception that model selection is about choosing the best model
 - For explanation one should be open to the possibility of there may be several (roughly) equally good explanatory models
 - For prediction one may want to do model averaging rather than model selection (expert opinion analogy)

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Donner party data

- Reasonable models/theories
 - 1. $logit[P(Y = 1|age)] = \beta_0 + \beta_1 age$
 - 2. $logit[P(Y = 1|fem)] = \beta_0 + \beta_2 fem$
 - 3. $logit[P(Y = 1|age, fem)] = \beta_0 + \beta_1 age + \beta_2 fem$
 - 4. $logit[P(Y = 1|age, fem)] = \beta_0 + \beta_1 age + \beta_2 fem + \beta_3 fem \cdot age$

Which model should we use?

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Model selection

What are you looking for?

- Model selection: One wants, given the sample, to choose a model that can describe the underlying distribution of the data
- But one only has limited information, namely the sample, and therefore one can not determine with complete certainty the underlying data generating mechanism
- Thus one looks for the most "likely" model, given your sample
- Competing models can be formally compared via
 - Nested models: Wald test, LRT
 - Nested and non-nested models: AIC (Akaike Information Criterion),
 BIC (Bayesian Information Criterion)
- Keep research question in mind!

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Information criteria

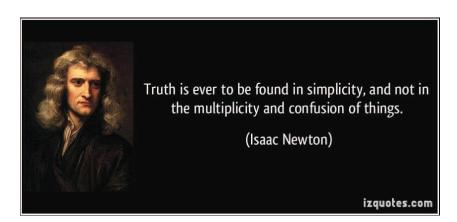
• AIC and BIC can be used to compare nested and non-nested models

$$\begin{aligned} \mathsf{AIC} &= & -2\log(\mathsf{LMAX}) + 2(\# \text{ of parameters}) \\ \mathsf{BIC} &= & -2\log(\mathsf{LMAX}) + \log(n)(\# \text{ of parameters}) \end{aligned}$$

- Penalty for complexity, i.e., for the number of parameters used
- Occam's razor: Other things being equal, simpler explanations are generally better than more complex ones

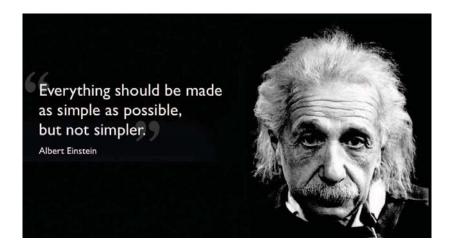
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Occam's razor



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Occam's razor



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Information criteria: AIC and BIC

- Smaller is better
- AIC and BIC are not equivalent. They have different characteristics and look for different models (different definitions of "best"). My personal choice: AIC
- AIC selects from a list of competing models the model that is "closest" to the underlying model
- "Closest" can be rigorously defined, namely, the model that minimizes the expected estimated Kullback-Leibler divergence cross-entropy

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Akaike information criterion: AIC

- A single AIC value is meaningless. AIC values are meaningful only when they are compared with other AIC values
- The Akaike-weights are easier to interpret: Posterior probability that the model is the "best" model in the Kullback-Leibler sense
- Suppose one has a list of R competing models/theories then
 - \bullet Find the model with the smallest $\mbox{AIC}_{\mbox{\scriptsize min}}$
 - For every model i, compute $\Delta_i = AIC_i AIC_{min}$
 - For every model i, compute the Akaike-weights

$$w_i = \frac{\exp(-\frac{1}{2}\Delta_i)}{\sum_{i=1}^R \exp(-\frac{1}{2}\Delta_i)}$$

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Donner party data: Model selection via AIC

Model selection

Rank	Covai	riates		AIC	Δ_i	Akaike–weights
3	age			118.02	3.15	0.115
4	fem			118.88	4.01	0.075
1	age	fem		114.88	0.00	0.559
2	age	fem	$age \cdot fem$	116.47	1.60	0.251

$$w_T = \exp\left(-\frac{0.00}{2}\right) + \exp\left(-\frac{1.60}{2}\right) + \exp\left(-\frac{3.15}{2}\right) + \exp\left(-\frac{4.01}{2}\right) = 1.7909$$

$$w_1 = \frac{\exp\left(-\frac{0.00}{2}\right)}{w_T} = \frac{1}{1.7909} = 0.559$$

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Donner party data: Model selection via AIC

Model selection

Rank	Cova	riates		AIC	Δ_i	Akaike–weights
3	age			118.02	3.15	0.115
4	fem			118.88	4.01	0.075
1	age	fem		114.88	0.00	0.559
2	age	fem	age \cdot fem	116.47	1.60	0.251

$$w_T = \exp\left(-\frac{0.00}{2}\right) + \exp\left(-\frac{1.60}{2}\right) + \exp\left(-\frac{3.15}{2}\right) + \exp\left(-\frac{4.01}{2}\right) = 1.7909$$

$$w_2 = \frac{\exp\left(-\frac{1.60}{2}\right)}{w_T} = \frac{0.4493}{1.7909} = 0.251$$

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Donner party data: Model selection via AIC

Model selection

Rank	Cova	riates		AIC	Δ_i	Akaike–weights
3	age			118.02	3.15	0.115
4	fem			118.88	4.01	0.075
1	age	fem		114.88	0.00	0.559
2	age	fem	$age \cdot fem$	116.47	1.60	0.251

$$w_T = \exp\left(-\frac{0.00}{2}\right) + \exp\left(-\frac{1.60}{2}\right) + \exp\left(-\frac{3.15}{2}\right) + \exp\left(-\frac{4.01}{2}\right) = 1.7909$$

$$w_3 = \frac{\exp\left(-\frac{3.15}{2}\right)}{w_T} = \frac{0.2070}{1.7909} = 0.115$$

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Donner party data: Model selection via AIC

Model selection

Rank	Cova	riates		AIC	Δ_i	Akaike–weights
3	age			118.02	3.15	0.115
4	fem			118.88	4.01	0.075
1	age	fem		114.88	0.00	0.559
2	age	fem	age \cdot fem	116.47	1.60	0.251

$$w_T = \exp\left(-\frac{0.00}{2}\right) + \exp\left(-\frac{1.60}{2}\right) + \exp\left(-\frac{3.15}{2}\right) + \exp\left(-\frac{4.01}{2}\right) = 1.7909$$

$$w_4 = \frac{\exp\left(-\frac{4.01}{2}\right)}{w_T} = \frac{0.1347}{1.7909} = 0.075$$

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Donner party data: Model selection via AIC

Model selection

Rank	Covariat	tes	AIC	Δ_i	Akaike–weights
3	age		118.02	3.15	0.115
4	fem		118.88	4.01	0.075
1	age fe	m	114.88	0.00	0.559
2	age fe	m age · fem	116.47	1.60	0.251

- Two models/theories, 1 and 2, seem to have some degree of support
- Some non-negligible level of model uncertainty
- A framework for scientific discussion: Which theory is more biologically plausible?

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Akaike-weights in R

```
> ## Fitting the models
> donner.list=list()
> donner.list[[1]]=glm(Outcome ~ Age,data=donner.na,family=binomial(link="logit"))
> donner.list[[2]]=glm(Outcome ~ fem,data=donner.na,family=binomial(link="logit"))
> donner.list[[3]]=glm(Outcome ~ Age + fem,data=donner.na,family=binomial(link="logit"))
> donner.list[[4]]=glm(Outcome ~ Age*fem,data=donner.na,family=binomial(link="logit"))
> donner.modnames <- c("Age", "Sex", "Age+Sex", "Age+Sex+Age:Sex")
>
```

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Akaike-weights in R

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Model averaging

Model averaging is one of several methods for making formal inference from multiple models (Burnham and Anderson 2002). This approach is quite different from standard variable selection methods where inference is made only from the selected model. Model averaging admits from the beginning of the analysis that there is substantial uncertainty as to what model is best and what combination of variables is important. On the contrary, selection methods such as stepwise selection pick a single best model. Inference is then conditional on this model and variables not in the model are, therefore, deemed unimportant. These are two very different approaches.

P. M. Lukacs et al., Ann Inst Stat Math (2010) 62:117-125

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Model average

- In presence of model uncertainty one may want to base inferences on several, similarly plausible, models instead of one single best model.
- One way of doing this is using a new type of model averaging estimator which averages $\hat{\beta}_i$ across several models.
- When calculating the model averaging estimator, one may consider only those models that contain the β_i parameter or, alternatively, all the models in the set of candidate models.
- The latter option is called the shrinkage estimator.

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Model average

• The model averaging estimator takes the form

$$\tilde{\beta}_i = \sum_{i=1} w_j \hat{\beta}_{ij},$$

where w_j is the Akaike weight of model g_j and $\hat{\beta}_{ij}$ is the MLE of β_i calculated using model g_j .

• When using the shrinkage estimator, i.e., if all models in the candidate set $\{g_1, \ldots g_R\}$ are used to compute the average, then $\hat{\beta}_{ij} \equiv 0$ if variable i is not included in model g_j .

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Model average

ullet The unconditional variance of $ilde{eta}_i$ is estimated as

$$\widehat{\mathsf{Var}}(\widetilde{eta}_i) = \sum_{i=1} w_j \left[\widehat{\mathsf{Var}}(\hat{eta}_{ij}|g_j) + (\hat{eta}_{ij} - \widetilde{eta}_i)^2 \right]$$

where w_j is the Akaike weight of model g_j and $\widehat{\beta}_{ij}$ and $\widehat{\text{Var}}(\widehat{\beta}_{ij}|g_j)$ are the MLE of β_i and its corresponding variance, calculated using model g_j .

• When using the shrinkage estimator, i.e., if all models in the candidate set $\{g_1, \dots g_R\}$ are used to compute the average, then $\widehat{\text{Var}}(\hat{\beta}_{ij}|g_j) \equiv 0$ if variable i is not included in model g_j .

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Model averaging in R

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Model averaging in R

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Donner party data: Conclusions

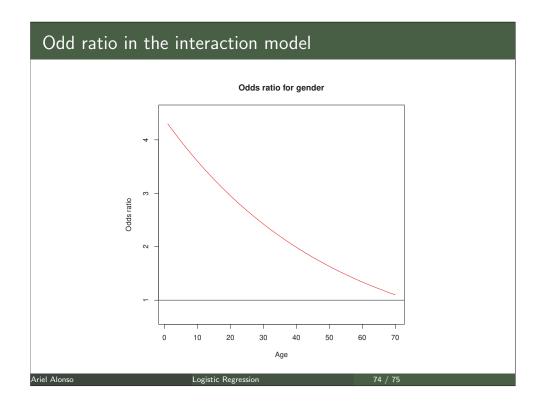
- Main effect model: Based on the data the estimated odds of survival for a woman is 3 ($\hat{OR} = e^{1067} \approx 3$) times larger than the corresponding odds of survival for a man of the same age, with a 95% CI for the odds ratio (1.15, 7.75), approximately
- There is *model selection uncertainty*: **Interaction model** has a relatively large Akaike-weight
- However, both models indicate that the odds of survival are larger for women than for men

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Odd ratio with the interaction model in R

```
> ## Gender odd ratio in the interaction model
>
> x=seq(1,70,0.01)
> y=exp(coef(m4)[3]+coef(m4)[4]*x)
>
> plot(x,y, type = "n", ylim=c(0.7, 4.5), xlab = "Age", ylab = "Odds ratio",
+ main="Odds ratio for gender")
> lines(x,y, lty = 1, col="red")
> abline(h=1)
```

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Donner party data: Conclusions

- It is important to note that this is an observational study (causal interpretations are therefore not justified)
- The sample was not drawn at random (inferences to a larger population are not strictly justified)

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