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## Extending the Linear Model

What is the problem?

- → So far, we exclusively considered continuous response variables. Now, we wish to extend this to binary and categorical response, proportions or counts!
  - This does not fit within the current framework
  - Counterexamples: → see next slides

We need some additional techniques which can deal with these types of situations. Depending on how the response variable is, there are several different approaches.

## Extending...: Example 1

### Logistic Regression, i.e. 0/1 response:

In human medicine, we are often interested in the question for how much "dose" of a medication we have an effect, i.e. a reduction in pain or symptoms.

#### Data:

Patients, where each one obtains some "dose" and as a response, either has a reduction (1), or not (0).

There may be some further predictors such as age, sex, ... that contribute towards predicting the response.

## Extending...: Example 1

### Logistic Regression, i.e. 0/1 response:

- A statistical model for this example takes into account that for a given "dose" resp. predictor configuration, we will only have an effect on some of the subjects, but not on all of them.
- We thus need to model the relation between the binary response and a number of predictors.

### The perhaps *simplest, but faulty approach* is:

$$P(Y_i = 1 \mid X) = \beta_0 + \beta_1 x_{i1} + ... + \beta x_{ip}$$

→ This will ultimately lead to probabilities beyond [0,1].

## Extending ...: Example 1

- We obtain a better model if we transform the response variable to a scale that ranges from minus to plus infinity.
- Usual choice is the so-called logit transformation:

$$p \mapsto \log(p/(1-p))$$

We obtain the **logistic regression model**:

$$\log\left(\frac{P(Y_i = 1 \mid X)}{1 - P(Y_i = 1 \mid X)}\right) = \beta_0 + \beta_1 x_{i1} + \dots + \beta_i x_{ip}$$

→ all fitted values are within [0,1].

## Extending...: Example 2

### **Poisson Regression**

What are predictors for the locations of starfish?

- → analyze the number of starfish at several locations, for which we also have some covariates such as water temperature, ...
- → the response variable is a count. The simplest model for this is a Poisson distribution.

We assume that the parameter  $\lambda_i$  at location i depends in a linear way on the covariates:

$$Y_i \mid X \sim Pois(\lambda_i)$$
, where  $\log(\lambda_i) = \beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}$ 

Extending...: Example 3

Log-Linear-Models

Question:

Prediction of a nominal response variable

### Example:

Which party does a person favor, depending on covariates such as education, age, sex, region, ...

- → such data can be summarized with contingency tables
- → and they can be modeled using log-linear models

### Generalized Linear Models

#### What is it?

- General framework for regression type modeling
- Many different response types are allowed
- Notion: the expected value of the response has a monotone relation to a linear combination of the predictors.

$$E[Y_i \mid X] = g(\beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip})$$

- Some further requirements on variance and density of Y
- → may seem complicated, but is very powerful!

## Binary Logistic Regression

#### What is it?

• Response  $Y_i \in \{0,1\}$ 

#### What do we need to take care of?

- Formulation of the model
- Estimation
- Inference
- Model diagnostics
- Model choice

## Example

Premature Birth, by Hubbard (1986)

 $Y_i \in \{0,1\}$  survival (1) /death (0) after premature birth.

#### **Predictors:**

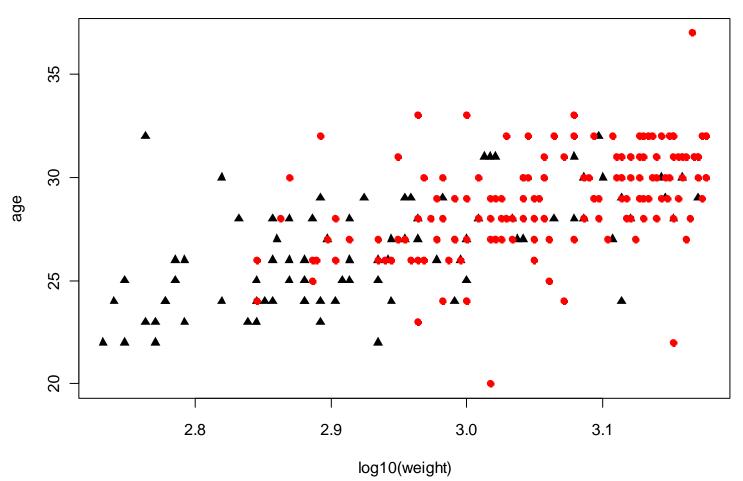
- weight (in grams) at birth
- age at birth (in weeks of pregnancy)
- apgar scores (vital function after 1 and 5 min)
- pH-value of the blood (breathing)

#### **Observations:**

- there are 247 instances

## **Example**

#### **Survival in Premature Birth**



## Logistic Regression Model

- $Y_i \in \{0,1\}$  has a Bernoulli distribution.
- The parameter of this distribution is  $p_i$ , the success rate

### Now please note that:

$$p_i = P(Y_i = 1 | X) = E[Y_i | X]$$

 $\rightarrow$  the most powerful notion of the logistic regression model is to see it as a model where we try to find a relation between the expected value of  $Y_i$  and the predictors!

**Important**:  $P(Y_i = 1) = \beta_0 + \beta_1 x_{i1} + ... + \beta_i x_{in}$  is no good here!

## Logit Transformation

**Goal**: mapping from  $[0,1] \mapsto (-\infty, +\infty)$ 

Logit transformation: 
$$g(p) = \log\left(\frac{p}{1-p}\right)$$

Interpretation: probabilities are mapped to logged odds ("Wettverhältnisse") which can then be modeled linearly.

$$\log \left( \frac{P(Y_i = 1 \mid X)}{1 - P(Y_i = 1 \mid X)} \right) = \beta_0 + \beta_1 x_{i1} + \dots + \beta_i x_{ip}$$

→ where is the error term?

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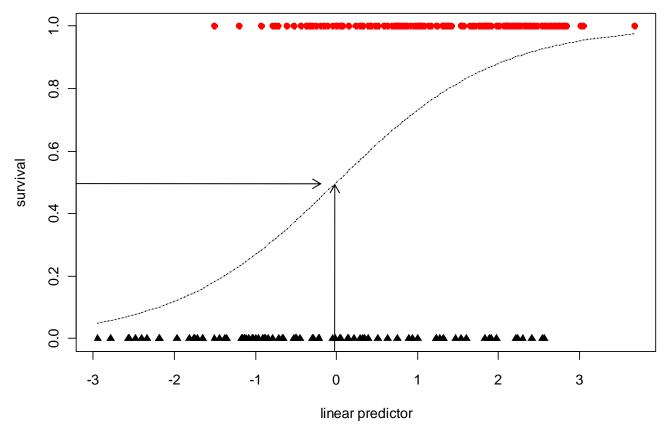
### Some Remarks

- For estimating the regression coefficients, we require the observations to be independent.
- There is no restriction for the predictors. They can be continuous, categorical, transformed, interactions, ...
- $\eta_i = \beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}$  is called the linear predictor
- $g(\cdot)$  is the link function, mapping between  $E[Y_i | X]$  and  $\eta_i$
- There are other (less important) link functions:
  - probit link
  - c-log-log link

### Survival vs. Linear Predictor

•  $g(P(Y=1|\log_{10}(weight), age)) = -33.97 + 10.17 \cdot \log_{10}(weight) + 0.14 \cdot age$ 

#### **Survival vs. Linear Predictor**



### **Estimation**

### Multiple linear regression:

→ minimize sum of squared residuals!
can be solved in closed form

### Logistic regression:

→ maximum likelihood approach!

leads to a non-linear equation system that needs to be solved with an iterative approach by weighted multiple linear regressions.

### **Important:**

→ seems like a very different paradigm, but is it?

## Interpretation of the Coefficients

→ see blackboard...

## Summary Output from R

```
> summary(glm(survival ~ I(log10(weight)) + age,
             family = "binomial", data = baby)
Deviance Residuals: ...
Coefficients: Estimate Std. Error z value Pr(>|z|)
(Intercept) -33.97108 4.98983 -6.808 9.89e-12 ***
I(log10(weight)) 10.16846 1.88160 5.404 6.51e-08 ***
             0.14742 0.07427 1.985 0.0472 *
age
Null deviance: 319.28 on 246 degrees of freedom
Residual deviance: 235.94 on 244 degrees of freedom
ATC: 241.94
```

### Inference: Individual Parameter Tests

### **Multiple Linear Regression:**

Gaussian errors  $\rightarrow \hat{\beta}_i$  are normally distributed

### **Logistic Regression:**

There are no errors, variability arises from Bernoulli distribution

The regression coefficients  $\hat{\beta}_j$  are only approximately normally distributed with a covariance matrix V that can be derived from the coefficients.

Hence: 
$$Z = \frac{\hat{\beta}_j - \beta_j}{\sqrt{\hat{V}_{jj}}} \sim N(0,1)$$

### Inference: Global Tests with GLMs

There are three tests, two can be done with logistic regression:

#### Goodness-of-fit test

- based on comparing against the saturated model
- not suitable for non-grouped, binary data

### Comparing two nested models

- likelihood ratio test leads to deviance differences
- test statistics has an asymptotic Chi-Square distribution

#### Global test

- comparing versus an empty model with only an intercept
- this is a nested model, take the null deviance

### Goodness-of-Fit

### **Multiple Linear Regression:**

Sum of Squared Residuals

### **Logistic Regression:**

Residual Deviance

$$D(y, \hat{p}) = -2\sum_{i} (y_i \log(\hat{p}_i) + (1 - y_i) \log(1 - \hat{p}_i))$$

- based on the log-likelihood
- in principle: comparison against fully saturated model
- for logistic regression, there is no formal test here

## Comparing Nested Models

Model 1: small model S, with q parameters

Model 2: big model B, with p parameters

### **Null hypothesis and test statistic:**

$$H_0: \beta_{q+1} = \beta_{q+2} = ... = \beta_p = 0$$

$$2(ll^{(B)} - ll^{(S)}) = D(y, \hat{p}^{(S)}) - D(y, \hat{p}^{(B)})$$

#### Distribution of the test statistic:

$$D^{(S)} - D^{(B)} \sim \chi_{p-q}^2$$

## Example with drop1()

#### **Question:**

- where is the difference to the summary output?
- it exists, though it's not obvious and asymptotically vanishes

### AIC and Variable Selection

#### **General remark:**

All comparison between models of different size can also be done using the AIC criterion. Not only in logistic regression, but also here.

#### The criterion:

$$AIC = D(y_i, \hat{p}) + 2p$$

#### Variable selection:

- stepwise approaches as with multiple linear regression
- factor variables need to be treated the right way!

### **Null Deviance**

#### **Smallest model:**

- The smallest model is without predictors, only with intercept
- Fitted values will all be equal to  $\hat{\pi}_0$
- Our best fit (F) and the smallest model (0) are nested

### A global test:

$$2(ll^{(F)} - ll^{(0)}) = D(y, \hat{p}^{(0)}) - D(y, \hat{p}^{(F)})$$

### Example and "Quick Check": → see blackboard...

Null deviance: 319.28 on 246 degrees of freedom

Residual deviance: 235.94 on 244 degrees of freedom

## Model Diagnostics

### Diagnostics are:

- in principle as important with logistic regression as they are with multiple linear regression models
- again based on differences between fitted & observed values
- → we now have to take into account that the variances are not equal for the different instances.
- → we have to come up with novel types of residuals:

#### Pearson and Deviance residuals

### Pearson Residuals

Take the difference between observed and fitted value and divides by an estimate of the standard deviation:

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

- $\rightarrow R_i^2$  is the contribution of the ith observation to the Pearson statistic for model comparison.
- → It is important to note that Pearson residuals exceeding a value of two in absolute value warrant a closer look

### Deviance Residuals

Take the contribution of the ith observation to the log-likelihood, i.e. the chi-square statistic for model comparison.

$$d_i = (y_i \cdot \log(\hat{p}_i) + (1 - y_i) \cdot \log(1 - \hat{p}_i))$$

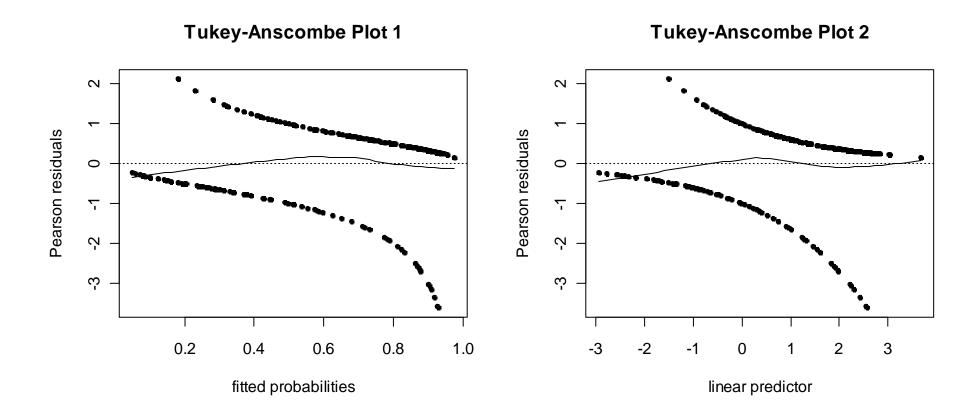
For obtaining a well interpretable residual, we take the square root and the sign of the difference between true and fitted value:

$$D_i = sign(y_i - \hat{\pi}_i) \cdot \sqrt{d_i}$$

- → deviance residuals > 2 warrant a closer look.
  - the distribution of the deviance residuals is not known.

## Tukey-Anscombe Plot

Remark: sometimes studentized residuals are used!



## Tukey-Anscombe Plot

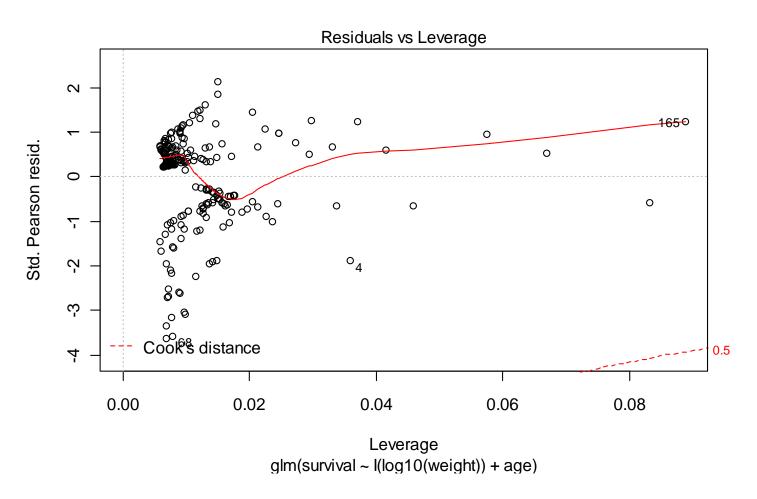
The Tukey-Anscombe plots in R are not perfect. Better use:

```
xx <- predict(fit, type="response")
yy <- residuals(fit, type="pearson")
loess.smooth(xx, yy, family="gaussian", pch=20)
abline(h=0, lty=3)</pre>
```

#### Reasons:

- using a non-robust smoother is a must
- different types of residuals can be used
- on the x-axis: probs or linear predictor

## More Diagnostics



## Binomial Regression Models

Concentration in log of mg/l	Number of insects n_i	Number of killed insects y_i
0.96	50	6
1.33	48	16
1.63	46	24
2.04	49	42
2.32	50	44

- $\rightarrow$  for the number of killed insects, we have  $Y_i \sim Bin(n_i, p_i)$
- > we are mainly interested in the proportion of insects surviving
- → these are grouped data: there is more than 1 observation for a given predictor setting

### Model and Estimation

The goal is to find a relation:

$$p_i = P(Y_i = 1 \mid X) \sim \eta_i = \beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip}$$

We will again use the logit link function such that  $\eta_i = g(p_i)$ 

$$\log\left(\frac{p_{i}}{1-p_{i}}\right) = \beta_{0} + \beta_{1}x_{i1} + ... + \beta_{p}x_{ip}$$

Here, $p_i$  is the expected value  $E[Y_i / n_i]$ , and thus, also this model here fits within the GLM framework. The log-likelihood is:

$$l(\beta) = \sum_{i=1}^{k} \left[ \log \binom{n_i}{y_i} + n_i y_i \log(p_i) + n_i (1 - y_i) \log(1 - p_i) \right]$$





## Fitting with R

We need to generate a two-column matrix where the first contains the "successes" and the second contains the "failures"

> fit <- glm(killsurv~conc, family="binomial")</pre>

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## **Summary Output**

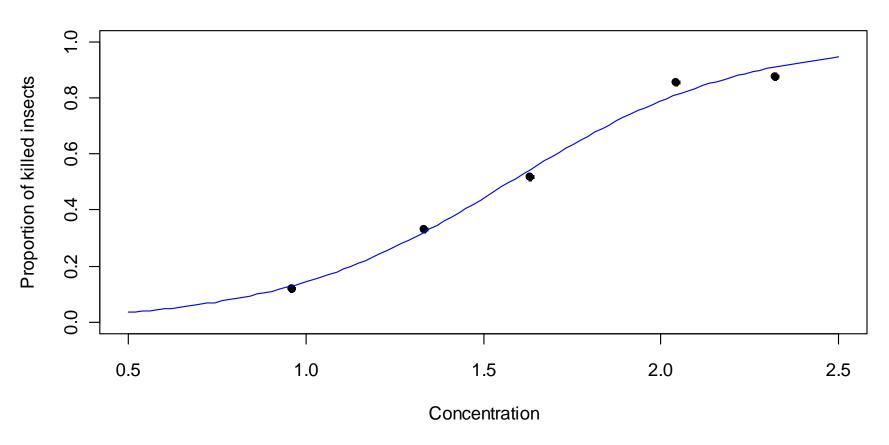
The result for the insecticide example is:

Null deviance: 96.6881 on 4 degrees of freedom Residual deviance: 1.4542 on 3 degrees of freedom

AIC: 24.675

## Proportion of Killed Insects

#### **Insecticide: Proportion of Killed Insects**



## Global Tests for Binomial Regression

For GLMs there are three tests that can be done:

#### Goodness-of-fit test

- based on comparing against the saturated model
- not suitable for non-grouped, binary data

### Comparing two nested models

- likelihood ratio test leads to deviance differences
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#### Global test

- comparing versus an empty model with only an intercept
- this is a nested model, take the null deviance

### Goodness-of-Fit Test

→ the residual deviance will be our goodness-of-fit measure!

**Paradigm**: take twice the difference between the log-likelihood for our current model and the saturated one, which fits the proportions perfectly, i.e.  $\hat{p}_i = y_i / n_i$ 

$$D(y, \hat{p}) = 2\sum_{i=1}^{k} \left[ y_i \log \left( \frac{y_i}{\hat{y}_i} \right) + (n_i - y_i) \log \left( \frac{(n_i - y_i)}{(n_i - \hat{y}_i)} \right) \right]$$

Because the saturated model fits as well as any model can fit, the deviance measures how close our model comes to perfection.

### Evaluation of the Test

### **Asymptotics:**

If  $Y_i$  is truly binomial and the  $n_i$  are large, the deviance is approximately  $\chi^2$  distributed. The degrees of freedom is:

$$k-(\# of predictors)-1$$

> pchisq(deviance(fit), df.residual(fit), lower=FALSE)
[1] 0.69287

### **Quick and dirty:**

 $Deviance \gg df$ : → model is not worth much. More exactly: check  $df \pm 2\sqrt{df}$ 

 $\rightarrow$  only apply this test if at least all  $n_i \ge 5$ 

## Overdispersion

What if  $Deviance \gg df$  ???

### 1) Check the structural form of the model

- model diagnostics
- predictor transformations, interactions, ...

### 2) Outliers

- should be apparent from the diagnostic plots

### 3) IID assumption for $p_i$ within a group

- unrecorded predictors or inhomogeneous population
- subjects influence other subjects under study

## Overdispersion: a Remedy

We can deal with overdispersion by estimating:

$$\hat{\phi} = \frac{X^2}{n-p} = \frac{1}{n-p} \cdot \sum_{i=1}^{n} \frac{(y_i - n_i \hat{p}_i)^2}{n_i \hat{p}_i (1 - \hat{p}_i)}$$

This is the sum of squared Pearson residuals divided with the df

### Implications:

- regression coefficients remain unchanged
- standard errors will be different: inference!
- need to use an F-test for comparing nested models

## Results when Correcting Overdispersion

```
> phi <- sum(resid(fit)^2)/df.residual(fit)</pre>
> phi
[1] 0.4847485
> summary(fit, dispersion=phi)
           Estimate Std. Error z value Pr(>|z|)
(Intercept) -4.8923 0.4474 -10.94 <2e-16 ***
       3.1088 0.2701 11.51 <2e-16 ***
conc
(Dispersion parameter taken to be 0.4847485)
Null deviance: 96.6881 on 4 degrees of freedom
Residual deviance: 1.4542 on 3 degrees of freedom
AIC: 24.675
```

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For GLMs there are three tests that can be done:

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## Testing Nested Models and the Global Test

For binomial regression, these two tests are conceptually equal to the ones we already discussed in binary logistic regression.

→ We refer to our discussion there and do not go into further detail here at this place!

### **Null hypothesis and test statistic:**

$$\begin{split} H_0: \beta_{q+1} &= \beta_{q+2} = \dots = \beta_p = 0 \\ 2 \Big( l l^{(B)} - l l^{(S)} \Big) &= D \Big( y, \hat{p}^{(S)} \Big) - D \Big( y, \hat{p}^{(B)} \Big) \end{split}$$

#### Distribution of the test statistic:

$$D^{(S)} - D^{(B)} \sim \chi_{p-q}^2$$