Marcel Dettling

Institute for Data Analysis and Process Design

Zurich University of Applied Sciences

marcel.dettling@zhaw.ch

http://stat.ethz.ch/~dettling

ETH Zürich, December 2, 2013

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: \rightarrow 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:

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

\rightarrow 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*:

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

 \rightarrow 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 assumes a Poisson as the conditional distribution.

We assume that the parameter λ_i at location *i* depends in a linear way on the covariates:

$$y_i | X \sim Pois(\lambda_i)$$
, 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, ...

 \rightarrow such data can be summarized with contingency tables \rightarrow 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 responses' conditional expectation has a monotone relation to a linear combination of the predictors. $E[Y_i | X] = g(\beta_0 + \beta_1 x_{i1} + ... + \beta_p x_{ip})$
- 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.

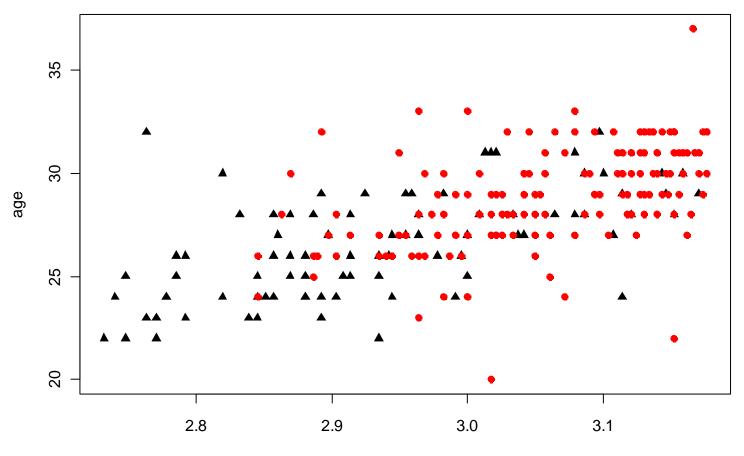
Predictors:

- 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:

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

→ 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 conditional expected value of y_i and the predictors!

Important: $P(y_i = 1) = \beta_0 + \beta_1 x_{i1} + ... + \beta x_{ip}$ 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.

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

\rightarrow where is the error term?

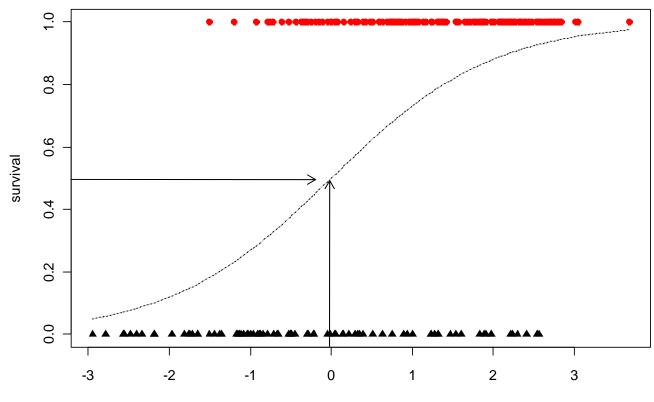
...

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 from $E[y_i | X]$ to η_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:

 \rightarrow seems like a very different paradigm, but is it?

Interpretation of the Coefficients

→ see blackboard...

Summary Output from R

Deviance Residuals: ...

Coefficients:	Estimate S	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	* * *
age	0.14742	0.07427	1.985	0.0472	*
Null deviance: 319.28 on 246 degrees of freedom					
Residual deviance: 235.94 on 244 degrees of freedom					
AIC: 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 hierarchical 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 Hierarchical Models

Model 1: small model S, with q parameters

Model 2: big model B, with p parameters

Null hypothesis and test statistic:

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

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

Distribution of the test statistic:

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

Example with drop1()

<pre>> drop1(fit, test="Chisq")</pre>						
Single term deletions						
Model: survival ~ I(log10(weight)) + age						
	Df	Deviance	AIC	LRT	Pr(Chi)	
<none></none>		235.94	241.94			
I(log10(weight))	1	270.19	274.19	34.247	4.855e-09	* * *
age	1	239.89	243.89	3.948	0.04694	*

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.
- \rightarrow 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:

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

- → R_i^2 is the contribution of the *i*th 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 *i*th observation to the log-likelihood, i.e. the chi-square statistic for model comparison.

$$d_{i} = (y_{i} \cdot \log(\hat{p}_{i}) + (1 - y_{i}) \cdot \log(1 - \hat{p}_{i}))$$

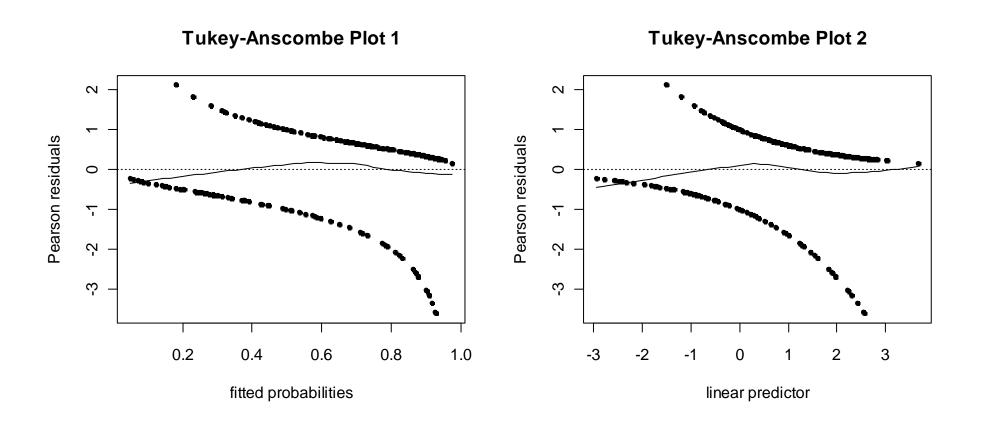
For obtaining a well interpretable residual, we take the square root and the sign of the difference between true and fitted value:

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

- \rightarrow 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

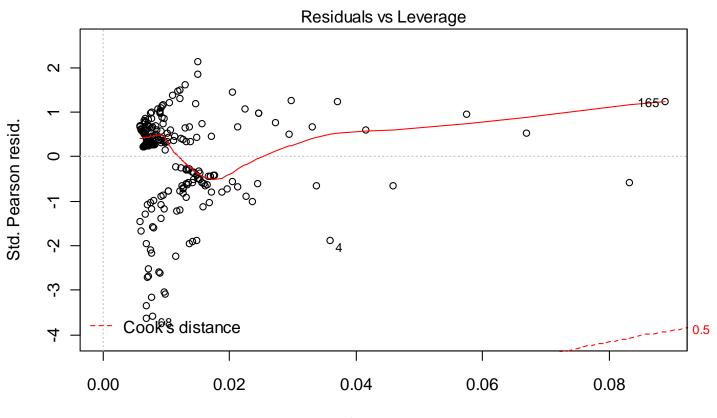
The Tukey-Anscombe plots in R are not perfect. Better use:

```
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



Leverage glm(survival ~ l(log10(weight)) + age)

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 $y_i \sim Bin(n_i, p_i)$

- \rightarrow 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:

$$p_i = P(y_i = 1 | X) \sim \eta_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip}$$

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

$$\log\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip}$$

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:

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

Marcel Dettling, Zurich University of Applied Sciences

zh aw

Zurich University of Applied Sciences

Fitting with R

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

	killed	surviv
[1,]	6	44
[2,]	16	32
[3,]	24	22
[4,]	42	7
[5,]	44	6

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

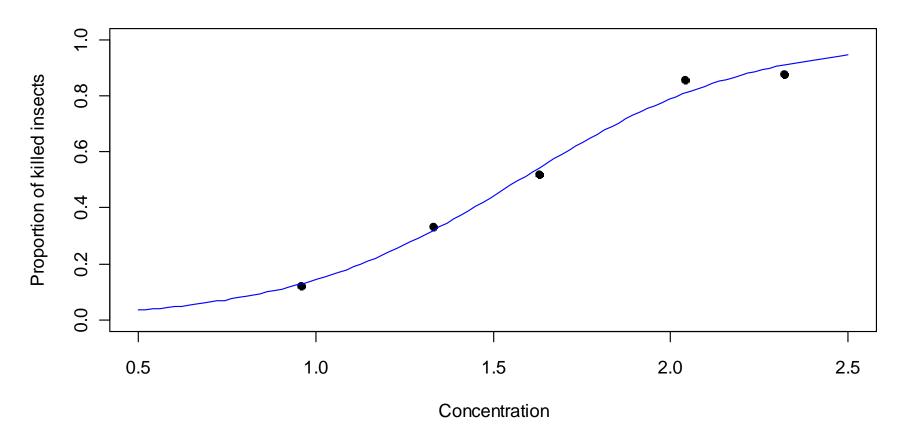
Summary Output

The result for the insecticide example is:

```
> summary(glm(killsurv ~ conc, family = "binomial")
```

```
Coefficients:
Estimate Std. Error z value Pr(>|z|)
(Intercept) -4.8923 0.6426 -7.613 2.67e-14 ***
conc 3.1088 0.3879 8.015 1.11e-15 ***
----
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 hierarchical 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 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 χ^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 $df \pm 2\sqrt{df}$

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

Marcel Dettling, Zurich University of Applied Sciences

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 *** conc 3.1088 0.2701 11.51 <2e-16 ***

(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

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 hierarchical 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

Testing Hierarchical Models / 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:

$$H_{0}: \beta_{q+1} = \beta_{q+2} = \dots = \beta_{p} = 0$$

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

Distribution of the test statistic:

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