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, October 14, 2013

Model Extensions

So far, simple linear regression was considered as fitting a straight line into a xy-scatterplot. While this is correct, it does not reflect the full potential of linear regression. With creative use of variable transformations, many more possibilities open.

Example: Automobile Braking Distance



We have data from 26 test drives with differing speed. The goal was to estimate the braking behavior of a certain type of tires. The data are displayed on the next slide...

Braking Distance: Data

Braking Distance vs. Speed	brdist	speed	obs	
	1.60	19.96	1	
Ŭ	Q	2.54	24.97	2
0	- 20	2.81	26.97	3
		3.58	32.14	4
Ē	ce [m] ⊤	4.59	35.24	5
		6.11	39.87	6
•	ing Distanc 30	7.91	44.62	7
		8.76	48.32	8
D C		10.12	52.18	9
20 III	raki 20	11.62	55.72	10
	Ê	13.57	59.44	11
ę	- 10	15.45	63.56	12
• •				
	0 -	51.09	111.97	24
20 40 60 80 100		50.69	115.88	25
Speed [km/h]		57.77	120.35	26

.

120

• .

Braking Distance: Fitting a Straight Line



Braking Distance: Facts

Conclusions from the residual plots:

• The straight line has a systematic error and does not reflect the true relation between speed and braking distance. From physics, we know that a parabola is more appropriate.

 $Distance_i = \beta_0 + \beta_1 \cdot Speed_i^2 + E_i$

resp. $y_i = \beta_0 + \beta_1 \cdot x'_i + E_i$, where $x'_i = x_i^2 = Speed_i^2$

• Please note that this is a simple linear regression problem. There is only one single predictor and the coefficients $\hat{\beta}_0, \hat{\beta}_1$ can and need to be estimated with the LS algorithm by taking partial derivatives and setting them to zero.

Braking Distance: Distance vs. Speed^2

> fit <- lm(weg ~ I(speed^2))</pre>



Curvilinear Regression

Simple linear regression offers more than fitting straight lines! We can fit any curvilinear relation with the LS algorithm. Some examples include:

• $y_i = \beta_0 + \beta_1 \cdot \ln(x_i) + E_i$

•
$$y_i = \beta_0 + \beta_1 \cdot \sqrt{x} + E_i$$

•
$$y_i = \beta_0 + \beta_1 \cdot x^{-1} + E_i$$

We are using $x'_i = \ln(x_i)$, $x'_i = \sqrt{x_i}$, bzw. $x'_i = (x_i)^{-1}$. In this form, it is obvious that all these are simple linear regression problems that can be solved via LS.

 \rightarrow **BUT...** see next slide

Braking Distance: Remarks

Curvilinear Models are often inadequate in practice:

• In our braking distance example, we should also consider the reaction time. This is a multiple regression model:

$$Distance_{i} = \beta_{0} + \beta_{1} \cdot Speed_{i} + \beta_{2} \cdot Speed_{i}^{2} + E_{i}$$

- Often, the variance/scatter of the errors is non-constant.
 In many examples, it increases with increasing.
- In many applications, the polynomial degree is not dictated by theorie, but needs to be estimated, too:

$$y_i = \beta_0 + \beta_1 \cdot x^{\beta_2} + E_i$$

Infant Mortality vs. Per-Capita Income



Infant Mortality vs. Per-Capita Income

The Fitted Hyperbolic Regression Line



Infant Mortality vs. Per-Capita Income

Residuals from Hyperbolic Fit



Residuals vs. Predictor

The Problem and the Solution

The hyperbolic fit shows some systematic error and is **not** the correct relation between mortality and income. We could try to estimate a power law such as:

$$y_i = \beta_0 + \beta_1 \cdot x_i^{\beta_2} + E_i$$

However, this problem is **non-linear** in the parameter β_2 and cannot be solved with the LS algorithm. Moreover, the error **variance** is **non-constant**.

A simple yet very useful trick solves the problem:

$$y_i' = \log(y_i), \ x_i' = \log(x_i)$$

For details, see the next slide and the blackboard...

The Log-Transformation Helps!



Model and Coefficients

If a straight line is fitted on the log-log-scale,

$$y' = \beta'_0 + \beta_1 \cdot x' + E'$$
, where $y' = \log(y)$, $x' = \log(x)$,

this means fitting the following relation on the original scale:

$$y = \beta_0 \cdot x^{\beta_1} \cdot E$$

The meaning of the parameter β_1 is as follows:

If *x*, i.e. the income increases by 1%, then *y*, i.e. the mortality decreases by $\hat{\beta}_1 = 0.56\%$. In other words: β_1 characterizes the relative change in *y* per unit of relative change in *x*.

The Fitted Relation



Infant Mortality vs. Per-Capita Income

Fitted Values and Intervals

• For predicting the y-value on the original scale, we can just re-exponentiate to invert the log-transformation and hence:

 $\hat{y} = \exp(\hat{y}')$

 Beware: this is an estimate of the conditional median, but not the conditional mean E[y | x]. If we require unbiased estimation, we need to use a correction factor :

 $\hat{y} = \exp(\hat{y}' + \hat{\sigma}_E^2 / 2)$

• The confidence and prediction intervals are easy:

 $[l,u] \rightarrow [\exp(l), \exp(u)]$

Conditional Mean and Median



Infant Mortality vs. Per-Capita Income

Confidence and Prediction Interval



What to do if y=0 and/or x=0?

- We can only take logarithms if x, y > 0. In cases where the response and/or predictor takes negative values, we should not log-transform. If zero's occur, they need treatment.
- What do we do with either x = 0 or y = 0?
 - do never exclude such data points!
 - adding a constant value is allowed!
- What about the choice of the constant?
 - standard choice: c = 1
 - scale dependent, thus not recommended!
- \rightarrow Set c = smallest value > 0!

Another Example: Daily Cost in Rehab



Logged Response Model

We *transform* the *response* variable and try to explain it using a linear model with our previous predictors:

$$y' = \log(y) = \beta_0 + \beta_1 x + E$$

In the *original scale*, we can write the logged response model using the same predictors:

 $y = \exp(\beta_0) \cdot \exp(\beta_1 x) \cdot \exp(E)$

→ Multiplicative model

→ $E \sim N(0, \sigma_E^2)$, and thus, $\exp(E)$ has a lognormal distribution

Fit and Residuals after the Transformation



Original Scale: Fit and Prediction Interval



Interpretation of the Coefficients

Important: There is no back transformation for the coefficients to the original scale, but still a good interpretation

$$log(y) = \beta_0 + \beta_1 x + E$$

$$y = exp(\beta_0)exp(\beta_1 x)exp(E)$$

An increase by one unit in x would multiply the fitted value in the original scale with $exp(\beta_1)$.

→ Coefficients are interpreted multiplicatively!

When to Transform?

We have seen a few examples where a log-transformation of the response and/or the predictor yields a better fit. Some general rules about when to apply it:

- If the values are on a scale, that is **left-closed** (with 0 as the smallest possible value), but is **open** on the **right**.
- If the marginal distribution of the variable (as we can observe in a histogram) is clearly **right-skewed**.
- If the scatter, i.e. the magnitude of the uncertainty, increases with increasing value – be this due to theoretical considerations, or due to evidence in the data.

Transformations: Lynx Data



Lynx Trappings

Transformations: Lynx Data



Zurich Airport Data: Re-Evaluation

Both Pax and ATM are variables that only take values ≥ 0 . In our example, we do not observe any right-skewness, but we still try to apply the log-transformation:

 $ATM' = \log(ATM), Pax' = \log(Pax)$

It also has the advantage that the fit goes through (0/0).

```
> fit <- lm(Pax ~ ATM, data=unique2010)
> fit.log <- lm(log(Pax) ~ log(ATM), data=unique2010)
> fit.y.orig <- exp(fitted(fit.log)[order(unique2010$ATM)])
> plot(Pax ~ ATM, data=unique2010, pch=20)
> lines(sort(unique2010$ATM), fit.y.orig, col="blue")
> abline(fit, col="red")
```

The difference in the fitted line is only small, but important!

Zurich Airport Data: Re-Evaluation



Zurich Airport Data: Pax vs. ATM

We estimate $\hat{\beta}_1 = 1.655$. If ATM increases by 1% then Pax will increase by 1.655%.

This reflects that during high season, bigger airplanes are used, and the seat load factor is better.

Comparing the Residual Plots

