Chapter 7

Nonlinear Models

7.1 Nonlinear Regression Models

7.1.1 Linearization of the Model

– Often seemingly nonlinear models can be linearized and reparametrized into the form of generalized linear models.

– For example

(a)

$$\mu_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 \Longleftrightarrow \mu_i = \beta_0 + \beta_1 x_i + \beta_2 z_i + \beta_3 w_i, \tag{7.1}$$

where $x_i^2 = z_i, x_i^3 = w_i$.

(b)

$$\mu_i = e^{\beta_0} e^{\beta_1 x_{i1}} x_{i2}^{\beta_2} x_{i3}^{\beta_3} \Longleftrightarrow \log(\mu_i) = \beta_0 + \beta_1 x_{i1} + \beta_2 \log(x_{i2}) + \beta_3 \log(x_{i3}). \tag{7.2}$$

(c)

$$\mu_i = \sqrt{\left(\frac{1}{\beta_0 + \beta_1 x_i}\right)} \Longleftrightarrow \frac{1}{\mu_i^2} = \beta_0 + \beta_1 x_i. \tag{7.3}$$

(d)

$$\mu_i = \frac{\beta_1 x_i}{\beta_0 + x_i} \Longleftrightarrow \frac{1}{\mu_i} = \frac{\beta_0}{\beta_1 x_i} + \frac{1}{\beta_1} = \alpha_0 + \alpha_1 z_i, \tag{7.4}$$

where $z_i = \frac{1}{x_i}, \alpha_0 = \frac{1}{\beta_1}, \alpha_1 = \frac{\beta_0}{\beta_1}$.

7.1.2 Single Variable Nonlinear Regression Models

– Under normality, the model is called nonlinear model, if in the model equation

$$Y_i = h(x_i, \boldsymbol{\beta}) + \varepsilon_i, \qquad \varepsilon_i \sim N(0, \sigma^2). \tag{7.5}$$

the derivatives of the expected value $\mu_i = h(x_i, \boldsymbol{\beta})$ depends on the vector $\boldsymbol{\beta}$.

– Under normality, the maximum likelihood estimator $\hat{\boldsymbol{\beta}}$ is also nonlinear least squares estimator

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left(y_i - h(x_i, \boldsymbol{\beta})\right)^2. \tag{7.6}$$

– In practice, it may be hard to define the function $h(x_i, \boldsymbol{\beta})$, and the starting values in estimation process of $\boldsymbol{\beta}$.

– R includes so called self-starting nonlinear models for one explanatory variable, where the starting values are automatically calculated for the parameter function $\boldsymbol{\beta}$ in function $h(x_i, \boldsymbol{\beta})$.

Function	Equation, $m(x, \phi) =$
SSasymp	Asymptotic regression
	$\phi_1 + (\phi_2 - \phi_1)\exp[-\exp(\phi_3)x]$
`SSasympOff()`	Asymptotic regression with an offset
	$\phi_1\{1 - \exp[-\exp(\phi_2) \times (x - \phi_3)]\}$
`SSasympOrig()`	Asymptotic regression through the origin
	$\phi_1\{1 - \exp[-\exp(\phi_2)x]\}$
`SSbiexp()`	Biexponential model
	$\phi_1 \exp[-\exp(\phi_2)x] + \phi_3 \exp[-\exp(\phi_4)x]$
`SSfol()`	First-order compartment model
	$\frac{D\exp(\phi_1+\phi_2)}{\exp(\phi_3)[\exp(\phi_2)-\exp(\phi_1)]}\{\exp[-\exp(\phi_1)x] - \exp([-\exp(\phi_2)x]\}$
`SSfpl()`	Four-parameter logistic growth model
	$\phi_1 + \frac{\phi_2-\phi_2}{1+\exp[(\phi_3-x)/\phi_4]}$
`SSgompertz()`	Gompertz model
	$\phi_1 \exp(\phi_2 x^{\phi_3})$
`SSlogis()`	Logistic model
	$\phi_1/(1 + \exp[(\phi_2 - x)/\phi_3])$
`SSmicmen()`	Michaelis-Menten model
	$\phi_1 x/(\phi_2 + x)$
`SSweibull()`	Weibull model
	$\phi_1 + (\phi_2 - \phi_1)\exp[-\exp(\phi_3)x^{\phi_4}]$

Table 1: The self-starting functions available in R, from Pinheiro and Bates (2000, Appendix C). Tools are also available for users to write their own self-starting functions.

Example 7.1.

Consider the data in file Alba.txt.

```
> data<-read.table("Alba.txt", sep="\t", dec=".", header=TRUE)
> attach(data)
> head(data)
  Dose  Herbicide DryMatter
1    1 Glyphosate       4.7
2    1 Glyphosate       4.6
3    1 Glyphosate       4.1
4    1 Glyphosate       4.4
5    1 Glyphosate       3.2
6    1 Glyphosate       3.0


Data are from an experiment, comparing the potency of the two herbicides
glyphosate and bentazone in white mustard Sinapis alba.

Dose - a numeric vector containing the dose in g/ha.
Herbicide - a factor with levels Bentazone Glyphosate (the two herbicides applied).
DryMatter - a numeric vector containing the response (dry matter in g/pot).

Christensen, M. G. and Teicher, H. B., and Streibig, J. C. (2003)
Linking fluorescence induction curve and biomass in herbicide screening,
Pest Management Science, 59, 1303?1310.
```

Denote the variables as $Y =$ DryMatter and $X =$ Dose.

(a) Model the data by the models

(i) $\mu_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3$,

(ii) $\mu_i = e^{\beta_0} x_i^{\beta_1}$,

(iii) $\mu_i = \sqrt{\left(\frac{1}{\beta_0 + \beta_1 x_i}\right)}$.

(b) Consider also the models

(i) $\mu_i = \beta_0 + (\beta_1 - \beta_0) e^{(-e^{\beta_2} x_i)}$,

(ii) $\mu_i = \frac{\beta_1 x_i}{\beta_0 + x_i}$,

(iii) $\mu_i = \beta_0 e^{\beta_1 \beta_2^{x_i}}$.

(c) Consider modeling the data by the model

$$\mu_i = \beta_{0j} + (\beta_{1j} - \beta_{0j}) e^{(-e^{\beta_{2j}} x_i)},$$

where there are different parameters in categories of the grouping variable Herbicide.

7.1.3 Confidence and Prediction Intervals in Nonlinear Models

– Confidence intervals can be created by the following parametric bootstrap method.

PARAMETRIC BOOTSTRAP BASED METHOD - CONFIDENCE INTERVAL

1. Find the estimate $\hat{\boldsymbol{\beta}}$ and $\widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}})$.
2. Simulate $\hat{\boldsymbol{\beta}}_*$ from the normal distribution $N(\hat{\boldsymbol{\beta}}, \widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}}))$.
3. Find the estimates $\hat{\mu}_* = h(x_i, \hat{\boldsymbol{\beta}}_*)$.
4. Repeat M times the steps 1-3, and then determine $\alpha/2$ and $1-\alpha/2$ the quantiles of the simulated values $\hat{\mu}_*$.

– Prediction intervals can be created by the following parametric bootstrap method.

PARAMETRIC BOOTSTRAP BASED METHOD - PREDICTION INTERVAL

1. Find the estimate $\hat{\boldsymbol{\beta}}, \hat{\sigma}^2$, and $\widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}})$.
2. Simulate $\hat{\boldsymbol{\beta}}_*$ from the normal distribution $N(\hat{\boldsymbol{\beta}}, \widehat{\mathrm{Cov}}(\hat{\boldsymbol{\beta}}))$.
3. Find the estimates $\hat{\mu}_{f_*} = h(x_f, \hat{\boldsymbol{\beta}}_*)$.
4. Simulate y_{f_*} from the distribution $y_{f_*} \sim N(\hat{\mu}_{f_*}, \hat{\sigma}^2)$.
5. Repeat M times the steps 1-4, and then determine $\alpha/2$ and $1-\alpha/2$ the quantiles of the simulated values y_{f_*} .

Example 7.2.

Consider the previous example. Model the data by the model

$$\mu_i = \beta_{0j} + (\beta_{1j} - \beta_{0j})e^{(-e^{\beta_{2j}} x_i)},$$

where there are different parameters in categories of the grouping variable Herbicide. Create confidence and prediction intervals when $x_f = 50$ and interest is the category Bentazone.