stats545.3 Topics in nonlinear statistical models

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Contents

1 Introduction to nonlinear statistical models

1.1 The assumptions - and what goes wrong

$$\mathbf{y} \sim n\left(\mathbf{X}\beta, \sigma^2 I\right)$$

may be wrong.
Simple variance exceptions are easy to handle:

- $Vy_i = u_i\sigma^2$ where u_i are known
- $\Sigma_\mathbf{y} = \sigma^2 B$ where B is known
- $\Sigma_\mathbf{y}$ may contain "a few" unknown parameters

1.1.1 Details

The assumption

$$\mathbf{y} \sim n\left(\mathbf{X}\beta, \sigma^2 I\right)$$

consists of several components: Normality, independence, linearity in the mean and equal variances.

The following sections give some examples of cases where general violations of these assumptions are handled using general nonlinear models.

Consider first the simplest deviations, namely of the variance structure:

- If $Vy_i = u_i\sigma^2$ where u_i are known, then we can define $w_1 = 1/u_i$ and maximum likelihood is equivalent to $min_\mathbf{b} \sum_i w_i \left(\mathbf{y}_i - \mathbf{x}_i'\beta\right)^2$ where $\mathbf{x}_i'$ is the i'th row of $\mathbf{X}$. This is the traditional **weighted linear regression**.
- If $\Sigma_\mathbf{y} = \sigma^2\mathbf{B}$ where $\mathbf{B}$ is known, then we can write $\mathbf{B}^{-1} = \mathbf{L}\mathbf{L}'$ where $\mathbf{L}$ is lower triangular and define a new regression problem with $\tilde{\mathbf{y}} = \mathbf{L}'\mathbf{y}$, $\tilde{\mathbf{X}} = \mathbf{L}'\mathbf{X}$ and it follows that $E\tilde{\mathbf{y}} = \tilde{\mathbf{X}}\beta$, $V\tilde{\mathbf{y}} = \ldots = \sigma^2\mathbf{I}$ so ordinary least squares can be used to estimate the parameters and for uncertainty estimation in the revised regression problem.
- If $\Sigma_\mathbf{y}$ contains "a few" unknown parameters, then these can be estimated as a part of maximum likelihood estimation of all parameters.

1.2 Maximum likelihood

The MLE is usually a good estimator
Applies to very many estimation problems
Need to specify the complete likelihood function
Can take into account dependence, different variances, non-normality, nonlinear response etc

1.2.1 Details

the likelihood approach involves...

1.2.2 Examples

Example: Consider maximum likelihood estimation of the mean of the gamma density.

$$\ldots$$

$$\Rightarrow \hat{\mu} = \bar{y}$$

Example: Consider a model for the growth of fish.

The data set at http://notendur.hi.is/gunnar/kennsla/alsm/data/set121.dat contains measurements of individual fish, collected by the Marine Research Institute (http://www.hafro.is). The data include a column (aldur) containing the age of fish and the column (le) containing the length of the same fish.

The von Bertalanffy growth model can be fitted using the R commands

```
dat<-read.table("http://notendur.hi.is/~gunnar/kennsla/alsm/data/set121.dat",header=T)
le<-dat$le
a<-dat$aldur
fm<-nls(le~Linf*(1-exp(-K*(a-t0))),start=list(t0=0,Linf=80,K=0.25))
summary(fm)
```

Once the above commands have been issued, the summary command can be used:

```
> summary(fm)

Formula: le ~ Linf * (1 - exp(-K * (a - t0)))

Parameters:
     Estimate Std. Error t value Pr(>|t|)
t0   -0.23160    0.23739  -0.976 0.331683
Linf 91.22292   14.47924   6.300 8.72e-09 ***
K     0.15672    0.04414   3.550 0.000595 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 2.788 on 97 degrees of freedom

Number of iterations to convergence: 3
Achieved convergence tolerance: 6.375e-07
```

A different test can also be used to investigate whether $t_0 = 0$:

```
> fmR<-nls(le~Linf*(1-exp(-K*(a))),start=list(Linf=80,K=0.25))
> anova(fm,fmR)
Analysis of Variance Table

Model 1: le ~ Linf * (1 - exp(-K * (a - t0)))
Model 2: le ~ Linf * (1 - exp(-K * (a)))
  Res.Df Res.Sum Sq Df Sum Sq F value Pr(>F)
1     97     753.78
2     98     762.33 -1 -8.557  1.1012 0.2966
```

Note that the F-test and t-test are not the same in the nonlinear case. Both depend on linearity assumptions but in different ways.

1.3 Nonlinear least squares

Common model:

$$Ey_i = g(\mathbf{x_i}, \beta),\ 1 \leq i \leq n$$

Common estimation method:

$$min_\beta \sum_i (y_i = g(\mathbf{x_i}, \beta))^2$$

Also need to estimate uncertainty. Use Hessian or bootstrap.

1.3.1 Detail

A common nonlinear model to predict y_i-values is to assume some functional relationship:

$$Ey_i = g(\mathbf{x_i}, \beta),\ 1 \leq i \leq n$$

where β is a vector of unknown parameters.

A very common estimation method is nonlinea least squares:

$$min_\beta \sum_i (y_i = g(\mathbf{x_i}, \beta))^2 .$$

This leaves the question of how to estimate the uncertainty in the parameters.

2 Generalized linear models

2.1 The linear model - different formulation

2.1.1 Details

The traditional linear model with independent $y_1, y_2, \ldots, y_n$ can be written as follows

1. $y_i \sim n(\mu_i, V[y_i])$
2. $\mu_i = \eta_i$
3. $V[y_i] = \sigma^2$

where $\eta_i = \underline{x}_i' \underline{\beta}$.

2.2 The generalized linear model

2.2.1 Details

The generalized linear model with independent $y_1, y_2, \ldots, y_n$ can be defined by

1. $y_1, y_2, \ldots, y_n$ come from a member of the exponential family of distributions.
2. $g(\mu_i) = \eta_i$ for some monotone function g, where $\eta_i = \underline{x_i'\beta}$ and $V[y_i]$ may be a function of μ_i.

The function g is the **link function** and n_i is the **linear predictor**. (The link function links the mean to the linear predictor.)

The traditional linear model is a special case of this generalized linear model.

The **exponential family** consists of distributions with density (pdf or pnf) of the form

$$f(y;\theta,\phi) = e^{\frac{y\theta - b(\theta)}{a(\phi)} + c(y,\phi)} \; (*)$$

where a, b and c are functions which make this a density. Commonly, $a(\phi) = \frac{\phi}{w}$ where $w > 0$ is known and $\phi = V[y_i] = \sigma^2$.

2.2.2 Examples

Example 1 - The Gaussian Density

Consider the usual linear model

$$\mathbf{y} \sim n(\mathbf{X}\beta, \sigma^2 I)$$

Here, $y_i \sim n(\mu_i, \sigma^2)$ where $\mu_i = \mathbf{x}_i'\beta$ are independent and $g =$ identity. We need to verify that the Gaussian density is of the form (*), that is,

$$f(y;\theta,\phi) = e^{\frac{y\theta - b(\theta)}{a(\phi)} + c(y,\phi)}$$

This Gaussian density is

$$\begin{aligned} f(y;\mu,\sigma) &= \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-\mu)^2}{2\sigma^2}} \\ &= \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{y^2 - 2\mu y + \mu^2}{2\sigma^2}} \\ &= \exp\left(\frac{y\mu - \frac{1}{2}\mu^2}{\sigma^2} - \left(\frac{y^2}{2\sigma^2} + \frac{1}{2}\ln(2\pi\sigma^2) \right) \right) \end{aligned}$$

which is of the form (*) if we set

$\phi = \sigma^2$,

$\theta = \mu$,

$a(\phi) = \phi$, $b(\theta) = \frac{1}{2}\theta^2$ and

$c(y,\phi) = -\left(\frac{y^2}{2\phi} + \frac{1}{2}\ln(2\pi\phi) \right)$.

Example 2 - The Γ-Density

First write the gamma density in the form

$$f(y;\mu,r) = \frac{y^{r-1} e^{\frac{-ry}{\mu}}}{\Gamma(r)\left(\frac{\mu}{r}\right)^r} \qquad \text{with } y > 0$$

If e.g. $y_1, y_2, \ldots, y_n$ are independent with this density and $\mu_i = E[y_i] = g(\mathbf{x}_i'\beta)$, then this is a GLM since the density is from the exponential family:

$$f(y;\mu,r) = \exp\left(\frac{y/\mu - \ln(\mu)}{1/r} + (r-1)\ln(y) - \ln(\Gamma(r)) + r\ln(r)\right)$$

which is of the form (*) with

$\theta = \frac{1}{\mu}$,

$\phi = r$,

$a(\phi) = \frac{1}{\phi}$,

$b(\theta) = -\ln(\theta)$ and

$c(y,\phi) = (\phi - 1)\ln(y) - \ln(\Gamma(\phi)) + \phi\ln(\phi)$.

Here $g(\mu) = \frac{1}{\mu}$ is called the **canonical link**, but it is much more common to use $g(\mu) = \ln(\mu)$, e.g. in fisheries or other ecological applications.

Example 3

Consider estimating the mean under the gamma assumption. So assume we have independent $y_1, y_2, \ldots, y_n$ with density

$$\frac{y^{r-1}e^{-ry/\mu}}{\Gamma(r)\left(\frac{\mu}{r}\right)^r} \qquad \text{with } y > 0$$

The maximum likelihood estimator for μ is obtained by maximizing the likelihood function:

$$L(\mu,r) = \prod_{i=1}^{n} \frac{y_i^{r-1}e^{-ry_i/\mu}}{\Gamma(r)\left(\frac{\mu}{r}\right)^r}$$

or maximizing

$$\ln(L(\mu,r)) = -n\cdot\ln\left(\Gamma(r)\frac{1}{r^r}\right) - nr\cdot\ln(\mu) + (r-1)\sum_{i=1}^{n}\ln(y_i) - \frac{r}{\mu}\sum_{i=1}^{n} y_i$$

and now we solve

$$0 = \frac{d}{d\mu}\ln(L(\mu,r)) = -\frac{nr}{\mu} + \frac{r\sum_{i=1}^{n} y_i}{\mu^2}$$

$$\Rightarrow \qquad n\mu = \sum_{i=1}^{n} y_i$$

and we obtain

$$\hat{\mu} = \overline{y}$$

Note that here $Ey_i = \mu (= \alpha\beta)$, so $\hat{\mu}$ is unbiased.

2.3 Estimation: MLEs and deviances

2.3.1 Details

Parameters in a GLM include both $\underline{\beta}$ and ϕ. The elements of $\underline{\beta}$ can be estimated using maximum likelihood, but several approaches exist for this. The likelihood function is in general

$$L(\underline{\mu};\underline{y}) = \prod_{i=1}^{n} e^{\frac{y_i\theta_i - y(\theta_i)}{a(\phi)} + c(y_i,\phi)}$$

If we define

$$l(\underline{\mu},\underline{y}) := -2\ln\left(L(\underline{\mu};\underline{y})\right)$$

as a natural quantity to be minimized, then we can also define the <u>scaled deviance</u> by

$$D^*(\underline{y},\underline{\mu}) := l(\underline{\mu},\underline{y}) - l(\underline{y},\underline{y})$$

and the <u>deviance</u> is

$$D(\underline{y};\mu) := \phi D^*(\underline{y},\underline{\mu})$$

We note that

1. Minimizing D over $\underline{\beta}$ is equivalent to maximizing the likelihood function.
2. If $a(\phi) = \frac{\phi}{w}$ then D does not include ϕ.

For a given model, the <u>deviance for the model</u> is $D(\underline{y},\hat{\underline{\mu}})$ where

$$\hat{\mu}_i = g^{-1}(\hat{\eta}_i) = g^{-1}(\underline{x}_i'\hat{\underline{\beta}})$$

is the MLE, and this quantity only depends on the data - it does not involve unknown parameters $\left(\text{if } a(\phi) = \frac{ph}{w}\right)$.

2.3.2 Examples

Examples of distributions covered by the exponential family include the normal, gamma, Poisson and binomial. Common link functions include

Family	Link function
Gaussian	id
Gamma	ln (or inverse)
Binomial	logistic (or probit)
Poisson	ln

Example 4

Consider predicting a value between zero and one. Within a small interval the probability might be linear, but obviously an assumption of linearity will not hold across a wide range.

$$y_i \sim b(n = 1, p_i)$$

so $Ey_i = p_i$ and $Vy_i = p_i(1 - p_i)$.

A common link function is the logistic function

$$\eta = g(\mu) = \text{logit}(p) := \ln\left(\frac{p}{1-p}\right) = \mathbf{x}'\beta$$

with inverse

$$\frac{1}{1 - e^{-\mathbf{x}'\beta}} = \frac{1}{1 + e^{-\eta}}$$

We do not transform our data to do a linear regression (people used to do this until they came to realize the problems that this method entails).

The p.m.f. and likelihood

$$\prod_{i=1}^{n} p_i^{y_i}(1-p_i)^{1-y_i} = \prod_{i=1}^{n}\left(\frac{p_i}{1-p_i}\right)^{y_i}(1-p_i)$$

where each y_i is 0 or 1. Here

$$\begin{aligned} l(\mathbf{y}, \mathbf{p}) &= -2\ln\big(L(\mathbf{p}; \mathbf{y})\big) \\ &= -2\sum_{i=1}^{n}\big(y_i \ln(p_i) + (1 - y_i)\ln(1 - p_i)\big) \end{aligned}$$

and $\phi = 1$.

It turns out that there is a whole pile of numerical methods available for finding these values.

This was already done in the seventies. Back then, it was a big thing to do this with your shiny new computer (without a graphical user interface though), which ran interactive programs that did more or less all the work for you.

When you are transforming the data, then you get biased estimators, so our method here is a lot better!

Therefore, the general recommendation is, that if you have data fitting this kind of model, you really should use this model and not transform your data.

Example 5 - Poisson

$y_i \sim P(\lambda_i)$ are independent and usually $\ln(\lambda_i) = \mathbf{x}_i'\beta$. Here

$$L(\underline{\lambda}) = \prod_{i=1}^{n}\frac{\lambda_i^{y_i}e^{-\lambda_i}}{y_i!}$$

and

$$\begin{aligned} l(\mathbf{y}, \underline{\lambda}) &= -2\sum_{i=1}^{n} \ln\left(\frac{l_i^{y_i} e^{-\lambda_i}}{y_i!}\right) \\ &= -2\sum_{i=1}^{n} (y_i \ln(\lambda_i) - \lambda_i - \ln(y_i!)) \end{aligned}$$

and

$$\begin{aligned} D(\mathbf{y}, \hat{\underline{\lambda}}) &= l(\hat{\underline{\lambda}}, \mathbf{y}) - l(\mathbf{y}, \mathbf{y}) \\ &= -2\sum (y_i \ln(\hat{\lambda}_i) - \hat{\lambda}_i - y_i \ln(y_i) + y_i) \\ &= -2\sum \left(y_i \ln\frac{\hat{\lambda}_i}{y_i} + (y_i - \hat{\lambda}_i)\right) \end{aligned}$$

and this needs to be minimized to find $\hat{\underline{\beta}}$, where $\hat{\lambda}_i = e^{\mathbf{x}_i'\beta}$.

3 Likelihood ratio tests

3.1 The LRT

The **likelihood ratio test** of $H_0 : \beta = \beta_0$ vs $H_a : \beta \neq \beta_0$

$$\lambda = \frac{L(\hat{\beta}_0)}{L(\hat{\beta})}.$$

The test rejects for large values of λ.

3.1.1 Handout

The **likelihood ratio test** of $H_0 : \beta = \beta_0$ vs $H_a : \beta \neq \beta_0$ proceeds by computing the ratio between the likelihood function values, at the two points, $L(\beta_0)$ and $L(\hat{\beta})$. This is the ratio

$$\lambda = \frac{L(\hat{\beta}_0)}{L(\hat{\beta})}.$$

The test rejects for large values of Λ. Note that $\lambda = \lambda(y_1, \ldots, y_n)$ is a function of the data so the rejection region translates into a statement about the data.

$$\lambda(\mathbf{x}) = \frac{\sup_{\theta\in\Theta_0} L(\theta)}{\sup_{\theta\in\Theta} L(\theta)} = \frac{L(\theta_0)}{L(\hat{\theta})}.$$

Theorem: (Asymptotic distribution of the LRT–simple H_0) For testing $H_0 : \theta = \theta_0$ versus $H_1 : \theta \neq \theta_0$, suppose $x_1, \ldots, X_n$ are i.i.d. $f(x|\theta)$, $\hat{\theta}$ is the MLE for θ (and $f(x|\theta)$ satisfies the regularity conditions found in Miscellanea 10.6.2. in Casella and Berger). Then under H_0, as $n \to \infty$,

$$-2\log\lambda(\mathbf{X}) \xrightarrow{\mathcal{D}} \chi^2_1$$

4 Case study: Fisheries

4.1 Biological systems are typically nonlinear

- Growth
- Mortality

$\vdots$

-

so the models should be nonlinear

4.2 A relatively simple problem, ADAPT

The ADAPT assessment model

$$min_{N_{0,y},N_{a,0},q_a} \sum_{ay} w_{ay} \left(ln(I_{ay}) - ln(q_a N_{ay}) \right)^2$$
$$\text{w.r.t.} N_{a+1,y+1} = \left(N_{ay} e^{-M/2} - C_{ay} \right) e^{-M/2}$$

where M is fixed and the catches, C_{ay} are given as numbers by age and year.
But the weighting factors w_{ay} need to be specified.

4.3 Gadget biological components

4.3.1 Details

Core: Parametric forward simulation model

- Consumption: Suitability functions
- Mortality: Due to predation or other natural or fishing
- Growth: Can depend on consumption. Several growth update implementations
- Migration: Through migration matrices
- Maturation: Move from immature to mature stock component
- Spawning: Lose weight and generate yearclass
- Symmetric: All species implemented in same way - fleet is also a predator

4.4 Data are typically not Gaussian

- Length distributions
- Survey indices

⋮

-

Data from a normal distribution are actually very rare in fishery science.
Obvious modifications to assumptions such as the multinomial typically does not improve anything.

4.5 Nonlinearity is not an issue per se

- Use nonlinear minimisation algorithms for estimation
- Can handle a lot of unknown parameters
- Can in principle estimate variances using Hessian matrices or bootstrap

4.6 Consider each data set

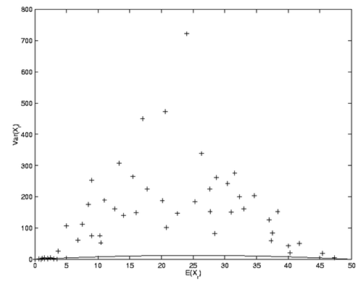
Look at single data sets and try to estimate true variances in each
Compare point estimates from each data set
Try to test formally whether results differ

4.7 Diagnostics for likelihood functions

Most likelihood functions can be verified, e.g. using Kolmogorov-Smirnov tests.
One should not be happy with a model which is rejected!

4.8 Likelihoods - Assumption

Take 50 fish from each station - compare with binomial



4.8.1 Details

Take 50 fish from each station - compare with binomial

4.9 Parsimony and flexibility

If data sources indicate different outcomes then the model is wrong!
Data are just data - they are not wrong.
Example: Catchability may vary in time and fleets may increase their catchability.
Need to add parameters until model is appropriately flexible. Notably add time series parameters...

5 Case study: Multispecies models for marine fish stocks

5.1 Combining data sets raises issues

- Weight given to each
- Do they all indicate the same model?

⋮

-

5.2 Several data sets means several likelihood components

In ADAPT

$$min_{N_{0,y},N_{a,0},q_a} \sum_{ay} w_{ay} \left(ln(I_{ay}) - ln(q_a N_{ay})\right)^2$$

$$\text{w.r.t.} N_{a+1,y+1} = \left(N_{ay} e^{-M/2} - C_{ay}\right) e^{-M/2}$$

the weighting factors w_{ay} need to be specified, since age groups are like data sets.
Complex data means means the components are not even of same form!

5.3 Length distributions

Multinomial?
Test assumptions using samples of survey stations, picking n fish from each.
Variance should be from binomial.
Covariance from multinomial.
Conclusion: Assumption fails very badly.

5.4 Effect of wrong variance assumptions

Linear model theory: Minor issue, just affects variance estimates, parameter estimates are still unbiassed.
But: If the base model is wrong for a small part of the data, may create havoc!

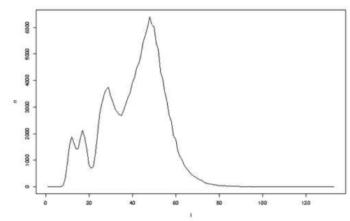
5.4.1 Examples

Example: Wrong weights in ADAPT

Weights on juveniles seem important - can drive entire assessment.

5.5 Likelihoods - Estimation procedure

Gadget is a statistical estimation model.
Internal dynamics are complex so deterministic forward projections are used.
Maximum likelihood estimation is used.



Length distributions are count data and are often assumed to come from a multinomial distribution, possibly with overdispersion.

5.5.1 Details

Estimation: (Negative log) likelihood functions

Gaussian, weighted

Multinomial

$$min_{\theta \in \mathbf{R}^n} \sum_k w_k l_k(\theta)$$

*N*ote: Given θ, can simulate. Now search for estimate giving best fit to weighted likelihood function.

5.6 Simple example of complexity problem

Take a simple problem

$$Y_{ij} \sim n(\alpha_i + \beta_i x_{ij}, \sigma_i^2), \quad j = 1, \ldots, n_i \;\; i = 1, 2,$$

but suppose we don't know the slopes are different, so fit

$$Y_{ij} \sim n(\alpha_i + \beta x_{ij}, \sigma_i^2), \quad j = 1, \ldots, n_i \;\; i = 1, 2,$$

5.7 Simple example of complex problem