

Nonlinear models

Bayesian statistics 8 – dynamic and nonlinear model fitting

Frédéric Barraquand (CNRS, IMB)

07/12/2021

Things that we learned the last time

- logistic regression with $y_i \sim \mathcal{B}(n, p_i)$ with
 $\text{logit}(p_i) = \log\left(\frac{p_i}{1-p_i}\right) = a + bx_i$ or $\gamma(x_i - \mu_x)$ which is equivalent to
 $p_i = \text{logistic}(a + bx_i) = \frac{\exp(a+bx_i)}{1+\exp(a+bx_i)} = \frac{1}{1+\exp(-(a+bx_i))}$

Things that we learned the last time

- logistic regression with $y_i \sim \mathcal{B}(n, p_i)$ with
 $\text{logit}(p_i) = \log\left(\frac{p_i}{1-p_i}\right) = a + bx_i$ or $\gamma(x_i - \mu_x)$ which is equivalent to
$$p_i = \text{logistic}(a + bx_i) = \frac{\exp(a + bx_i)}{1 + \exp(a + bx_i)} = \frac{1}{1 + \exp(-(a + bx_i))}$$
- “logistic ANOVA” $p_i = \text{logistic}(\alpha + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i})$. Here the logistic function maps $(-\infty, +\infty) \rightarrow [0, 1]$.

Things that we learned the last time

- logistic regression with $y_i \sim \mathcal{B}(n, p_i)$ with
 $\text{logit}(p_i) = \log\left(\frac{p_i}{1-p_i}\right) = a + bx_i$ or $\gamma(x_i - \mu_x)$ which is equivalent to
$$p_i = \text{logistic}(a + bx_i) = \frac{\exp(a+bx_i)}{1+\exp(a+bx_i)} = \frac{1}{1+\exp(-(a+bx_i))}$$
- “logistic ANOVA” $p_i = \text{logistic}(\alpha + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i})$. Here the logistic function maps $(-\infty, +\infty) \rightarrow [0, 1]$.
- We can also want to use the logistic function to *model a known curve*,
 $y_i = f(x_i) + \epsilon_i$ or $y_i = f(t_i) + \epsilon_i$

Organism growth basics: von Bertalanffy

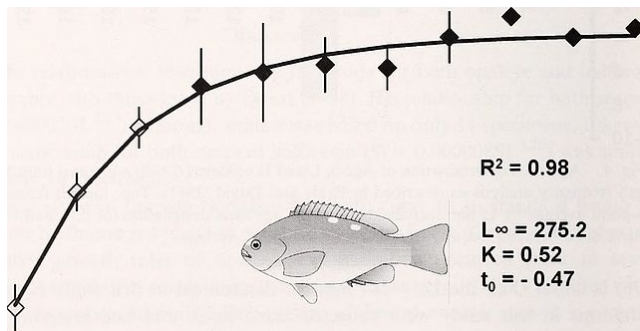


Figure 1: Von Bertalanffy growth curve fit to *Girella nigricans*

$$L(t) = L_{\infty}(1 - \exp(-k(t_i - t_0))) + \epsilon_i$$

Connection to dynamics

$$\frac{dL}{dt} = k(L_{\infty} - L)$$

Connection to dynamics

$$\frac{dL}{dt} = k(L_{\infty} - L)$$

We'll do for practical another example of organismal growth, Gompertz growth (Winsor PNAS 1932).

Dynamics

$$\frac{d \ln(L)}{dt} = k(\ln(L_{\infty}) - \ln(L))$$

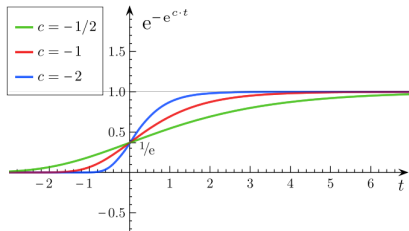
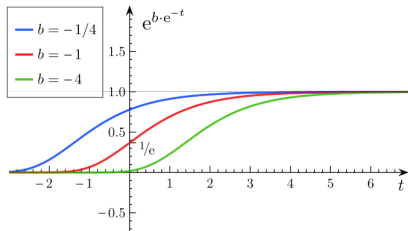
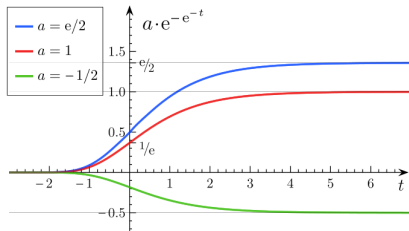
Solution

$$L(t) = ae^{-e^{b-ct}}$$

where $a = L_{\infty}e^1$, $b = kt_0$ and $c = k$.

Trick: note $I = \ln(L)$, solve von Bertalanffy for I , transform back.

The Gompertz growth curve is more logistic-like



Mathematical cousins of von Bertalanffy: modelling *saturation*

Monod function (microbiology) aka Michaelis-Menten (chemistry) aka Holling type II (ecology) aka ...

$$f(x) = \frac{ax}{b+x}$$

Another example of connection to dynamics: logistic population growth

N = population size (microbes, humans, wild boars, plants, . . .)

$$\frac{dN}{dt} = rN \left(1 - \frac{N}{K} \right)$$

And the solution is. . .

Another example of connection to dynamics: logistic population growth

N = population size (microbes, humans, wild boars, plants, ...)

$$\frac{dN}{dt} = rN \left(1 - \frac{N}{K}\right)$$

And the solution is...

$$N(t) = \frac{N_0 e^{rt}}{1 + N_0(e^{rt} - 1)/K}$$

If we use $t = 1, 2, 3, \dots$

$$N_1 = \frac{N_0 e^r}{1 + N_0(e^r - 1)/K}, N_2 = \frac{N_1 e^r}{1 + N_1(e^r - 1)/K}, \dots$$

aka Beverton-Holt model.

Two kinds of “noise” or stochasticity

Observational noise

$$y_{t+1} = N_{t+1} + \epsilon_t, \quad N_{t+1} = \frac{N_t e^r}{1 + N_t(e^r - 1)/K}, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

- The effect of ϵ_t does not accumulate. ϵ_1 does not affect N_8 .

Two kinds of “noise” or stochasticity

Observational noise

$$y_{t+1} = N_{t+1} + \epsilon_t, \quad N_{t+1} = \frac{N_t e^r}{1 + N_t(e^r - 1)/K}, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

- The effect of ϵ_t does not accumulate. ϵ_1 does not affect N_8 .

Process noise

$$N_{t+1} = \frac{N_t e^{r+\epsilon_t}}{1 + N_t(e^r - 1)/K}, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

- The effect of ϵ_t does accumulate. ϵ_1 *does* affect N_8 .

Two kinds of “noise” or stochasticity

Observational noise

$$y_{t+1} = N_{t+1} + \epsilon_t, \quad N_{t+1} = \frac{N_t e^r}{1 + N_t(e^r - 1)/K}, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

- The effect of ϵ_t does not accumulate. ϵ_1 does not affect N_8 .

Process noise

$$N_{t+1} = \frac{N_t e^{r+\epsilon_t}}{1 + N_t(e^r - 1)/K}, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

- The effect of ϵ_t does accumulate. ϵ_1 *does* affect N_8 .
- *autocorrelation* between N_t values. This is a *time series* model

Two kinds of “noise” or stochasticity

Observational noise

$$y_{t+1} = N_{t+1} + \epsilon_t, \quad N_{t+1} = \frac{N_t e^r}{1 + N_t(e^r - 1)/K}, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

- The effect of ϵ_t does not accumulate. ϵ_1 does not affect N_8 .

Process noise

$$N_{t+1} = \frac{N_t e^{r+\epsilon_t}}{1 + N_t(e^r - 1)/K}, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

- The effect of ϵ_t does accumulate. ϵ_1 *does* affect N_8 .
- *autocorrelation* between N_t values. This is a *time series* model
- Of course in real life you can have both (and sometimes it is hard to distinguish between the two)

Transforming this into a model we can fit

We need to have $y_t \sim \mathcal{D}(\text{[something]})$ to be able to fit a model in jags – the data must be observed. Let's take $y_t = \ln(N_t)$. Then the previous model writes

$$y_{t+1} = y_t + r + \epsilon_t - \ln(1 + \alpha N_t), \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

with $\alpha = (e^r - 1)/K$.

Transforming this into a model we can fit

We need to have $y_t \sim \mathcal{D}(\text{[something]})$ to be able to fit a model in jags – the data must be observed. Let's take $y_t = \ln(N_t)$. Then the previous model writes

$$y_{t+1} = y_t + r + \epsilon_t - \ln(1 + \alpha N_t), \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

with $\alpha = (e^r - 1)/K$.

Or again

$$y_{t+1} = y_t + r + \epsilon_t - \ln(1 + \alpha e^{y_t}), \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

Transforming this into a model we can fit

We need to have $y_t \sim \mathcal{D}(\text{[something]})$ to be able to fit a model in jags – the data must be observed. Let's take $y_t = \ln(N_t)$. Then the previous model writes

$$y_{t+1} = y_t + r + \epsilon_t - \ln(1 + \alpha N_t), \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

with $\alpha = (e^r - 1)/K$.

Or again

$$y_{t+1} = y_t + r + \epsilon_t - \ln(1 + \alpha e^{y_t}), \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

This equivalent to

$$y_{t+1} = f(y_t) + \epsilon_t \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2) \text{ i.i.d}$$

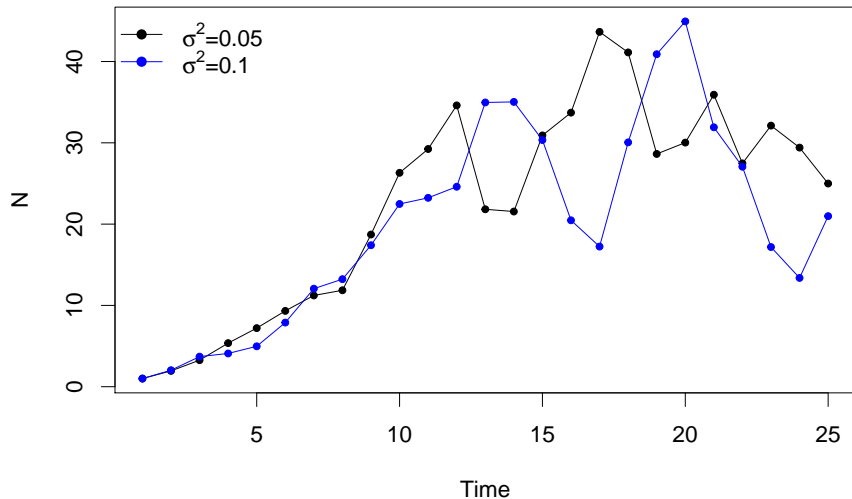
or again $y_{t+1}|y_t \sim \mathcal{N}(f(y_t), \sigma^2)$. We have our distribution!

Fitting the logistic model in discrete-time with process noise I

(you can fit the observational noise model with the solution $N(t)$ – you can't fit the process noise model solution, you have to fit the *dynamics*)

```
r=0.5
alpha=0.02
tmax=25
R=exp(r)
K=(exp(r)-1)/alpha
N_BH=N_BH1=rep(NA,tmax)
N_BH[1]=N_BH1[1]=1
for (t in 1:(tmax-1)){N_BH[t+1] =
  (exp(r+rnorm(1,0,sqrt(0.05))))*N_BH[t]/(1+alpha*N_BH[t])}
for (t in 1:(tmax-1)){N_BH1[t+1] =
  (exp(r+rnorm(1,0,sqrt(0.1))))*N_BH1[t]/(1+alpha*N_BH1[t])}
###
par(pch=20,cex=1.5)
plot(1:tmax,N_BH,type="o",ylim=range(c(N_BH,N_BH1)),xlab="Time",ylab="N")
lines(1:tmax,N_BH1,type="o",col="blue")
legend("topleft",c(expression(paste(sigma^"2","=0.05",sep="")),
  expression(paste(sigma^"2","=0.1",sep="))),
  col=c("black","blue"),lty=1,pch=16,bty="n")
```

Fitting the logistic model in discrete-time with process noise II



Let's fit the model

```
logistic.data <- list(logN = log(N_BH), tmax=tmax)

cat(file="logistic.growth.txt", "
model {
  r ~ dnorm(2, 0.01) ## prior on r
  alpha ~ dlnorm(1, 0.01) ## prior on alpha
  K <-(exp(r)-1)/alpha

  sigma ~ dunif(0.01,2)
  tau<-pow(sigma,-2)

  logN[1] ~ dnorm(0,1)
  N[1] <-exp(logN[1])

  #Likelihood
  for (t in 1:(tmax-1)){
    logNpred[t] <- logN[t]+ r - log(1 + alpha*N[t])
    logN[t+1] ~ dnorm(logNpred[t],tau)
    N[t+1] <- exp(logN[t+1])
  }
}
")
```

Running the model I

```
# Inits function
inits <- function(){list(r = rnorm(1, 0, 1),
                        alpha = rlnorm(1,0,1))}

# Parameters to estimate
params <- c("r", "alpha", "K", "sigma")

# MCMC settings
nc <- 3 ; ni <- 2000 ; nb <- 1000 ; nt <- 2

# Call JAGS, check convergence and summarize posteriors
out <- jags(logistic.data, inits, params, "logistic.growth.txt", n.thin = nt,
           n.chains = nc, n.burnin = nb, n.iter = ni)

## Compiling model graph
##   Resolving undeclared variables
##   Allocating nodes
## Graph information:
##   Observed stochastic nodes: 25
##   Unobserved stochastic nodes: 3
##   Total graph size: 183
##
## Initializing model
```

Running the model II

```
print(out, dig = 3)      # Bayesian analysis

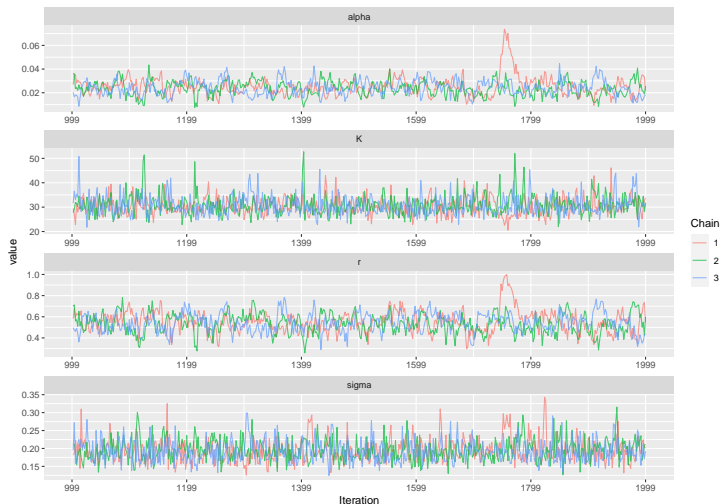
## Inference for Bugs model at "logistic.growth.txt", fit using jags,
## 3 chains, each with 2000 iterations (first 1000 discarded), n.thin = 2
## n.sims = 1500 iterations saved
##
```

	mu.vect	sd.vect	2.5%	25%	50%	75%	97.5%	Rhat	n.eff
## K	30.668	3.865	24.661	28.174	30.136	32.635	39.671	1.006	440
## alpha	0.024	0.007	0.013	0.020	0.024	0.028	0.038	1.009	230
## r	0.543	0.095	0.360	0.479	0.543	0.602	0.735	1.007	320
## sigma	0.194	0.031	0.144	0.172	0.190	0.213	0.269	1.002	820
## deviance	-10.380	2.795	-13.441	-12.409	-11.113	-9.177	-3.119	1.012	1500

```
##
## For each parameter, n.eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor (at convergence, Rhat=1).
##
## DIC info (using the rule,  $pD = \text{var}(\text{deviance})/2$ )
##  $pD = 3.9$  and  $DIC = -6.5$ 
## DIC is an estimate of expected predictive error (lower deviance is better).
```

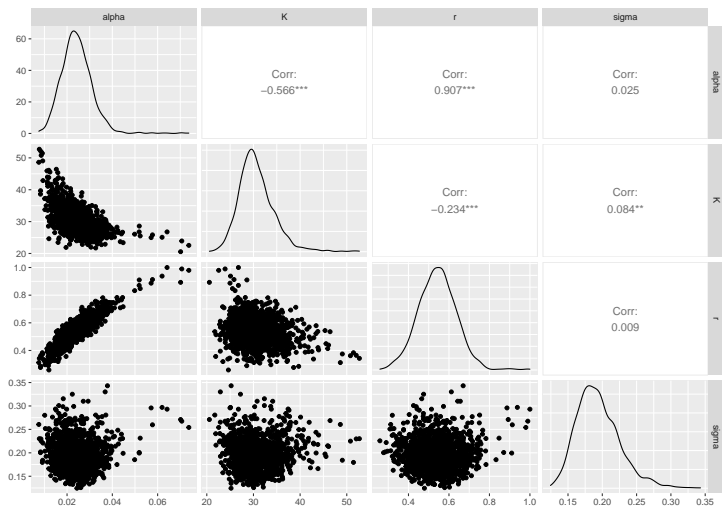
Showing traceplots

```
S<-ggs(as.mcmc(out)) #R2jags  
S<-filter(S,Parameter != "deviance")  
ggs_traceplot(S)
```



Showing correlations (r, K) and (r, α)

ggs_pairs(S)



How to interpret correlations in the posteriors

- Make some parameters difficult to interpret independently

How to interpret correlations in the posteriors

- Make some parameters difficult to interpret independently
- Here r is correlated to α but not really to K despite the fact that the formula K includes r in our JAGS code

How to interpret correlations in the posteriors

- Make some parameters difficult to interpret independently
- Here r is correlated to α but not really to K despite the fact that the formula K includes r in our JAGS code
- To maintain a nice curve that goes through the point cloud, r must be correlated with α .

How to interpret correlations in the posteriors

- Make some parameters difficult to interpret independently
- Here r is correlated to α but not really to K despite the fact that the formula K includes r in our JAGS code
- To maintain a nice curve that goes through the point cloud, r must be correlated with α .
- We'll see another example of this in the practical