Chapter 10. Statistical methodology for nonlinear partially observed Markov process models

Objectives

1. To introduce students to the `pomp` package
2. To explain how the components of a POMP model are encoded in this package
3. To give some experience in the use and manipulation of `pomp` objects.

Time series analysis via nonlinear partially observed Markov process (NL-POMP) models

Six problems of Bjornstad and Grenfell (Science, 2001): obstacles for ecological modeling and inference via nonlinear mechanistic models:

1. Combining measurement noise and process noise.
2. Including covariates in mechanistically plausible ways.
3. Continuous time models.
4. Modeling and estimating interactions in coupled systems.
5. Dealing with unobserved variables.
6. Modeling spatial-temporal dynamics.

Applications of NL-POMP models

- Modeling and inference via nonlinear mechanistic models arises throughout engineering, the sciences (social, biological and physical) and business.
- In finance, we considered a stochastic volatility example in Chapter 1.
- Infectious disease transmission dynamics can be highly nonlinear. Transmission arises when an infected individual contacts a susceptible individual, thus the rate of infections gets a nonlinear term:

$$\begin{aligned}&\text{Fraction of individuals infected}\\ &\quad\times\quad\text{Fraction of individuals susceptible to infection}\end{aligned}$$

- Each new infection depletes the pool of susceptible individuals. Without depletion of susceptibles, the fraction of individuals susceptible to infection is constant and the epidemic grows exponentially.
- Data on infectious diseases are generally limited to diagnosed cases. Much of the transmission dynamics cannot be directly observed.

Ecology and epidemiology as historical motivation for NL-POMP methods

- Infectious disease epidemiology has motivated developments in statistical methodology and software for NL-POMP models.
- Many other biological populations have similar nonlinearities: the population grows exponentially until limited by some constraint, such as a food resource or a predator. When the resource is used up, or the predator becomes abundant, the population crashes. Then a new cycle begins.
- Ecological systems and epidemiological systems have much in common. Disease systems can be relatively simple ecosystems with just two species: host and pathogen.

An algorithmic approach to inference for POMP models

Recall our notation for partially observed Markov process models. The latent process is $X_n = X(t_n)$ and we write $X_{0:N} = (X_0, \ldots, X_N)$. The observation at time t_n is modeled by a random variable Y_n. The one-step transition density, $f_{X_n|X_{n-1}}(x_n|x_{n-1};\theta)$, together with the measurement density, $f_{Y_n|X_n}(y_n|x_n;\theta)$ and the initial density, $f_{X_0}(x_0;\theta)$, specify the entire joint density via

$$f_{X_{0:N},Y_{1:N}}(x_{0:N},y_{1:N};\theta) = f_{X_0}(x_0;\theta)\prod_{n=1}^{N} f_{X_n|X_{n-1}}(x_n|x_{n-1};\theta)\, f_{Y_n|X_n}(y_n|x_n$$

The marginal density for $Y_{1:N}$, evaluated at the data, $y_{1:N}$, is

$$f_{Y_{1:N}}(y_{1:N};\theta) = \int f_{X_{0:N},Y_{1:N}}(x_{0:N},y_{1:N};\theta)\, dx_{0:N}.$$

Algorithmic notation matching the mathematical notation for POMP models

To think algorithmically, we define some function calls that provide **basic elements** specifying a POMP model.

- `rprocess()`: a draw from the one-step transition distribution, with density $f_{X_n|X_{n-1}}(x_n|x_{n-1};\theta)$.
- `dprocess()`: evaluation of the one-step transition density, $f_{X_n|X_{n-1}}(x_n|x_{n-1};\theta)$.
- `rmeasure()`: a draw from the measurement distribution with density $f_{Y_n|X_n}(y_n|x_n;\theta)$.
- `dmeasure()`: evaluation of the measurement density, $f_{Y_n|X_n}(y_n|x_n;\theta)$.
- This follows the standard R notation, for example we expect `rnorm` to draw from the normal distribution, and `dnorm` to evaluate the normal density.
- A general POMP model is fully specified by defining these basic elements.

Specifying our own POMP model

- The user will have to say what the basic elements are for their chosen POMP model.
- Algorithms can then use these basic elements to carry out inference for the POMP model.
- We will see that there are algorithms that can carry out likelihood-based inference for this general POMP model specification.

What does it mean for statistical methodology to be simulation-based?

- Simulating random processes can be easier than evaluating their transition probabilities.
- Thus, we may be able to write `rprocess()` but not `dprocess()`.
- **Simulation-based** methods require the user to specify `rprocess()` but not `dprocess()`.
- **Plug-and-play**, **likelihood-free** and **equation-free** are alternative terms for simulation-based.
- Much development of simulation-based statistical methodology has occurred in the past decade.

The **pomp** R package for POMP models

- `pomp` is an R package for data analysis using partially observed Markov process (POMP) models.
- Note the distinction: lower case `pomp` is a software package; upper case POMP is a class of models.
- `pomp` builds methodology for POMP models in terms of arbitrary user-specified `rprocess()`, `dprocess()`, `rmeasure()`, and `dmeasure()` functions.
- Following modern practice, most methodology in `pomp` is simulation-based, so does not require specification of `dprocess()`.
- `pomp` has facilities to help construct `rprocess()`, `rmeasure()`, and `dmeasure()` functions for model classes of scientific interest.
- `pomp` provides a forum for development, modification and sharing of models, methodology and data analysis workflows.
- `pomp` is available from CRAN or github.

Example: the Ricker model

- The Ricker model is a basic model in population biology. We start with a deterministic version and then add process noise and measurement error.
- The **Ricker equation** is a deterministic differential equation modeling the dynamics of a simple population, including population growth and resource depletion.

[R1] $$P_{n+1} = r\, P_n\, \exp(-P_n).$$

- Here, P_n is the population density at time $t_n = n$ and r is a fixed value (a parameter), related to the population's intrinsic capacity to increase.
- $P_n = \log(r)$ is an **equilibrium**, meaning that if $P_n = \log(r)$ then $P_{n+1} = P_{n+2} = \cdots = P_n$. Another equilibrium is $P_n = 0$.
- P is a **state variable**, r is a **parameter**.
- If we know r and the **initial condition** P_0, this deterministic Ricker equation predicts the future population density at all times.
- The initial condition, P_0 is a special kind of parameter, an **initial-value parameter**.

Adding stochasticity to the Ricker equation

- We can model process noise by making the growth rate r into a random variable.
- For example, if we assume that the intrinsic growth rate is log-normally distributed, P becomes a stochastic process governed by

[R2] $$P_{n+1} = r\,P_n\,\exp(-P_n + \varepsilon_n), \qquad \varepsilon_n \sim \text{Normal}(0, \sigma^2),$$

- Here, the new parameter σ is the standard deviation of the noise process ε.

Question 10.1. Does adding Gaussian noise mean we have a Gaussian latent process model? What does it mean to say that the model for $P_{0:N}$ described by equation [R2] is Gaussian?

Adding measurement error to the Ricker model

- Let's suppose that the Ricker model is our model for the dynamics of a real population.
- For most populations, outside of controlled experiments, we cannot know the exact population density at any time, but only estimate it through sampling.
- Let's model measurement error by treating the measurement y_n, conditional on P_n, as a draw from a Poisson distribution with mean $\phi\, P_n$. This corresponds to the model

[R3] $$Y_n | P_n \sim \text{Poisson}(\phi\, P_n).$$

- The parameter ϕ is proportional to the sampling effort.

Writing the Ricker model as a POMP model

- For our standard definition of a POMP model $(X_{0:N}, Y_{0:N})$, we can check that equations [R2] and [R3] together with the parameter P_0 define a POMP model with

$$X_n = P_n \tag{1}$$
$$Y_n = Y_n \tag{2}$$

- Following the usual POMP paradigm, P_n is a true but unknown population density at time t_n.

Working with the Ricker model in pomp

- The R package pomp provides facilities for modeling POMPs, a toolbox of statistical inference methods for analyzing data using POMPs, and a development platform for implmenting new POMP inference methods.
- The basic data-structure provided by pomp is the object of class pomp, alternatively known as a pomp object.
- A pomp object is a container that holds real or simulated data and a POMP model, possibly together with other information such as model parameters, that may be needed to do things with the model and data.
- Let's see what can be done with a pomp object.
- First, if we haven't already, we must install pomp. The package needs access to code compilers to operate properly so you should check the installation instructions at
  `https://kingaa.github.io/pomp/install.html`

- For the following, we also load some other packages.

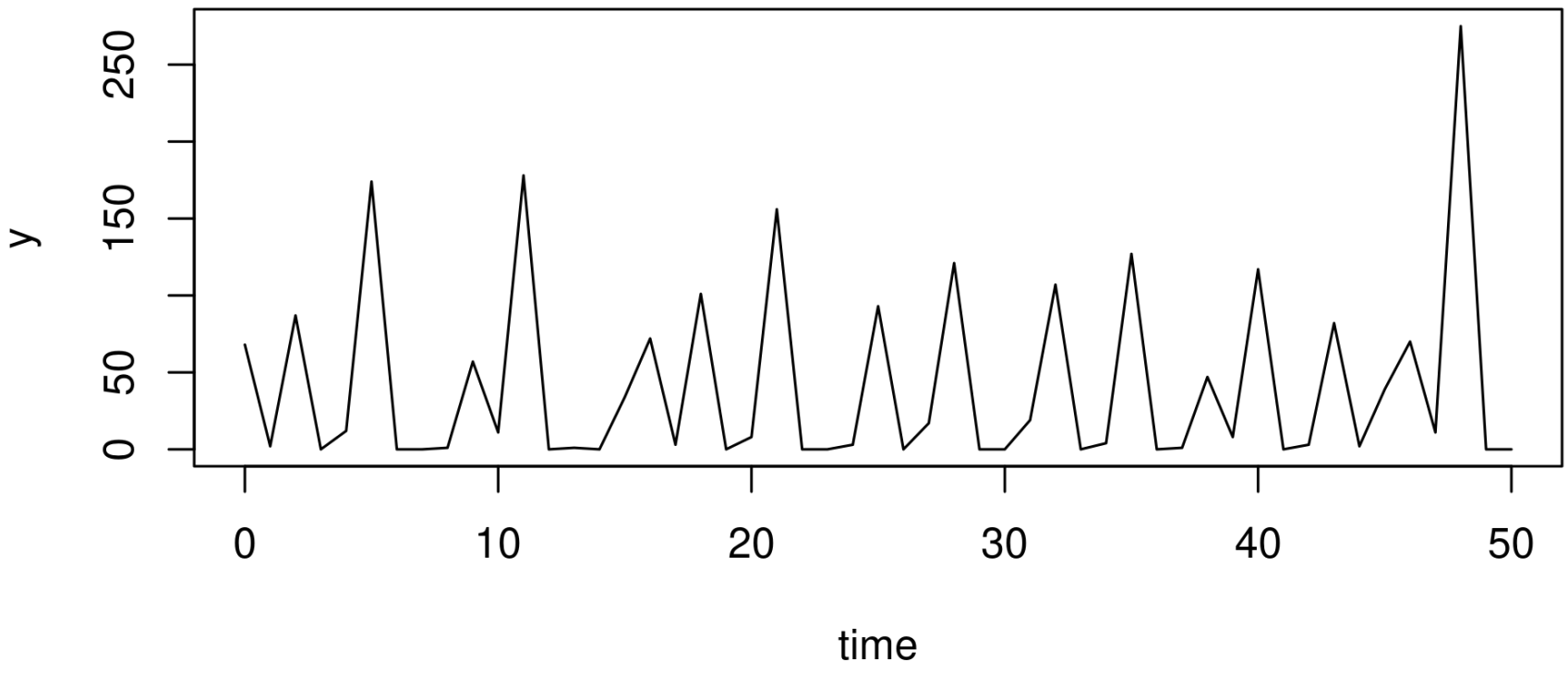
```
set.seed(594709947L)
require(ggplot2)
require(plyr)
require(reshape2)
require(pomp)
```

- A pre-built `pomp` object encoding the Ricker model comes included with the package. Load it by

```
ricker <- ricker()
```

We can plot the data:

```
plot(ricker)
```



- We can simulate from the model:

```
simulated_ricker <- simulate(ricker)
```

- What kind of object have we created?

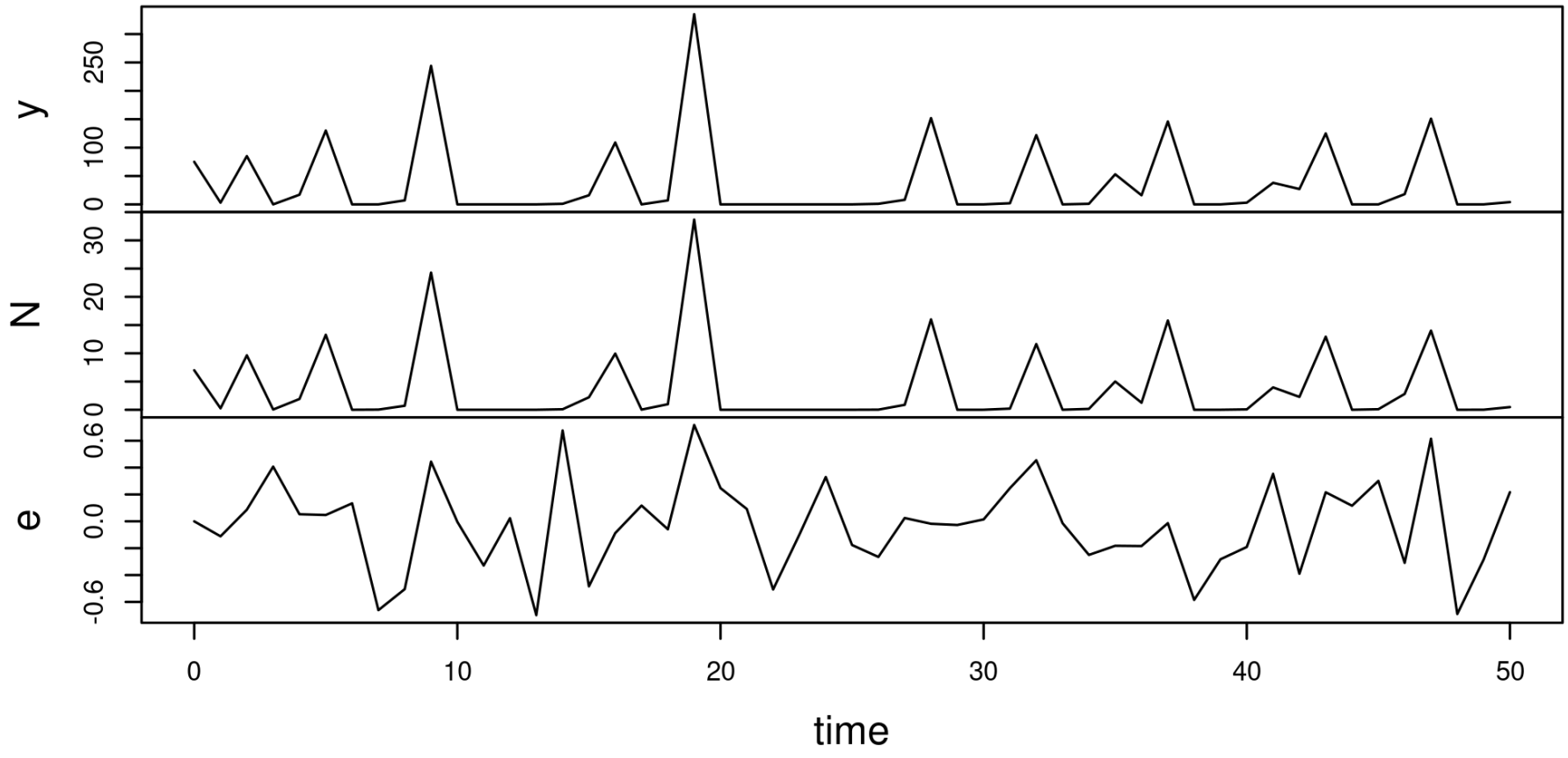
```
class(simulated_ricker)

## [1] "pomp"
## attr(,"package")
## [1] "pomp"
```

What is a generic function?

- How does the concept of a **generic function** fit in with the following related concepts,
- **object-oriented programming**
- assigning a **class** to an object.
- **overloading** of functions or operators.
- **inheritance** between classes, when one class extends another.
- How does object-oriented programming work in R? How is this similar or different from any other environment in which you have seen object-oriented programming?
- For current purposes, we don't need to be experts in object-oriented programming in R. However, we should be familiar with some R object-orientated basics.

- **S3 classes** (`http://adv-r.had.co.nz/OO-essentials.html#s3`)
- **S4 classes** (`http://adv-r.had.co.nz/S4.htm`)
- We should be able to recognize when code we are using employs S3 and S4 classes.
- We should know where to turn to for help if we find ourselves needing to know more details about how these work.
- `pomp` uses the S4 class system, so that system is of more immediate relevance. Many older R packages use S3 classes.

```
plot(simulated_ricker)
```



- This `pomp` representation uses `N` for our variable `P_n`

Question 10.2. Why do we see more time series in the simulated `pomp` object?

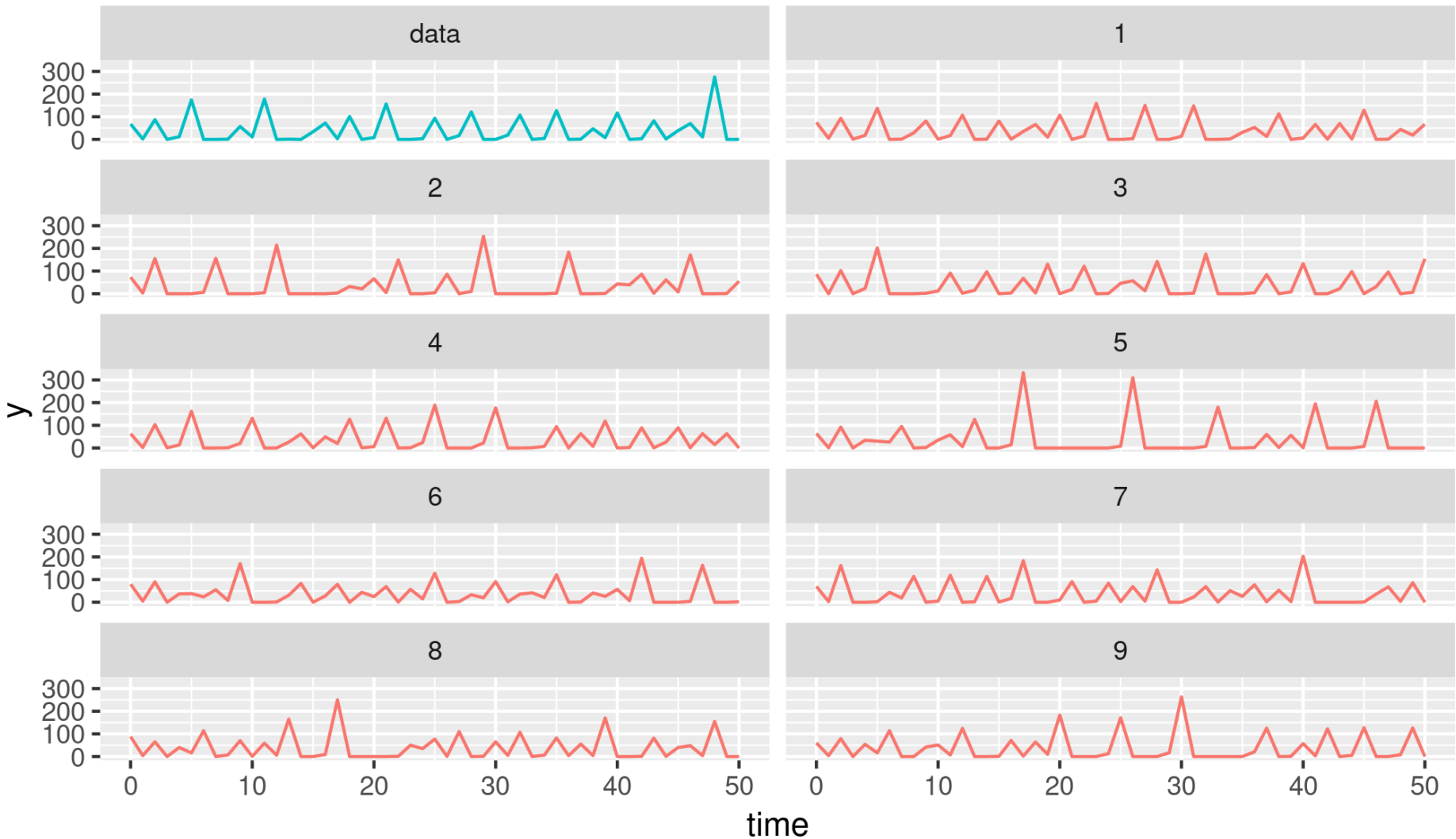
Different formats for simulation

- We can turn a pomp object into a data frame:

```
y <- as.data.frame(ricker)
head(y,3)

##   time  y
## 1    0 68
## 2    1  2
## 3    2 87

head(simulate(ricker,format="data.frame"))

##   time .id             N         e   y
## 1    0   1 7.000000e+00 0.0000000  85
## 2    1   1 4.326721e-01 0.4163146   1
## 3    2   1 1.406521e+01 0.1141514 147
## 4    3   1 7.566248e-04 0.4348591   0
## 5    4   1 4.084348e-02 0.1893917   0
## 6    5   1 1.794869e+00 0.0237836  21
```

- We can also run multiple simulations simultaneously:

```
x <- simulate(ricker,nsim=9,format="data.frame",include.data=TRUE)
ggplot(data=x,aes(x=time,y=y,group=.id,color=(.id=="data")))+
  geom_line()+guides(color=FALSE)+
  facet_wrap(~.id,ncol=2)
```

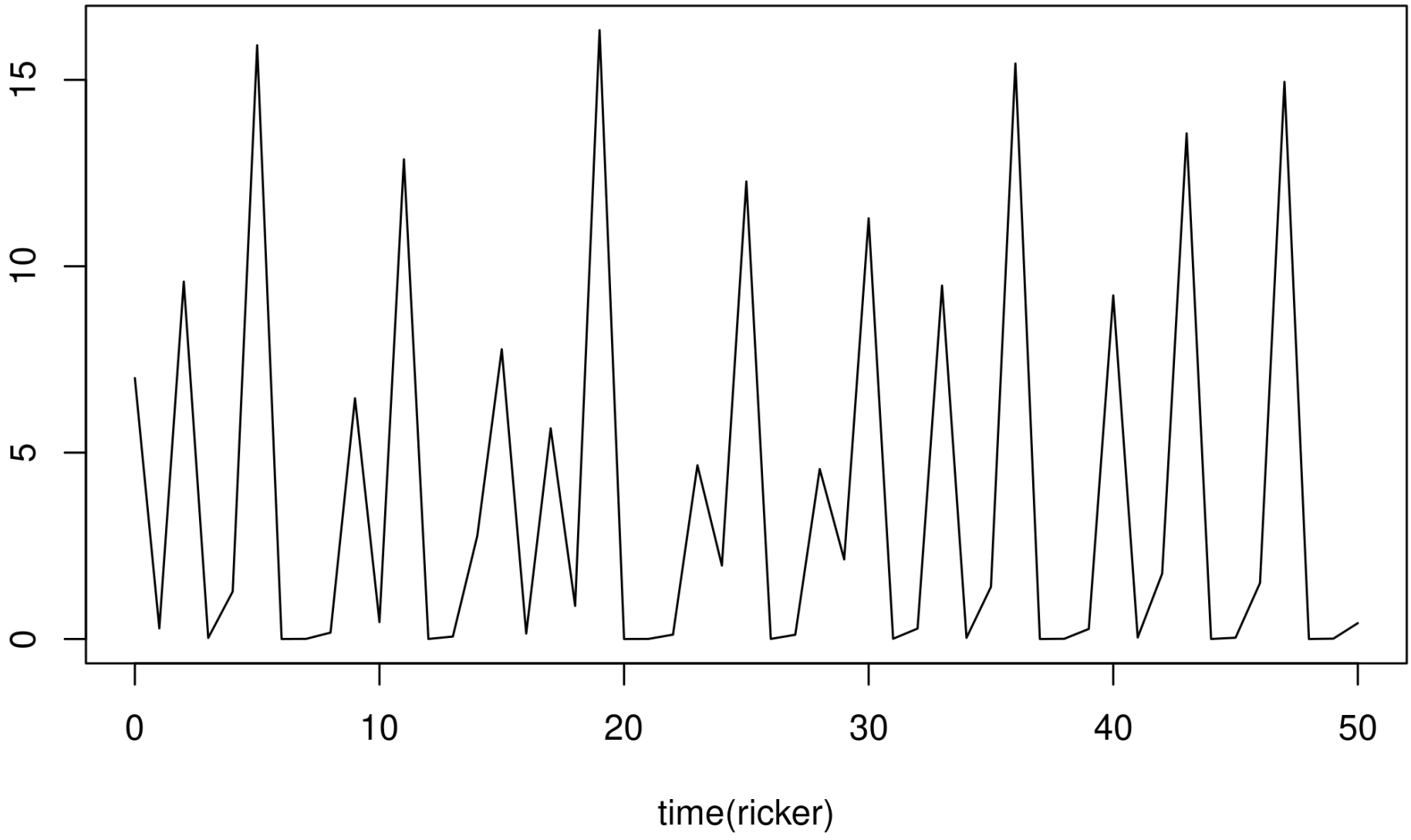


The deterministic skeleton

- The **deterministic skeleton** is a version of the POMP model without process noise.
- It is generated by `trajectory()`.

```
y <- trajectory(ricker)
dim(y)

## [1]  2  1 51

dimnames(y)

## $variable
## [1] "N" "e"
##
## $rep
## NULL
##
## $time
## NULL
```

```
plot(time(ricker),y["N",1,],type="l")
```



Working with model parameters I

- `ricker` has parameters associated with it:

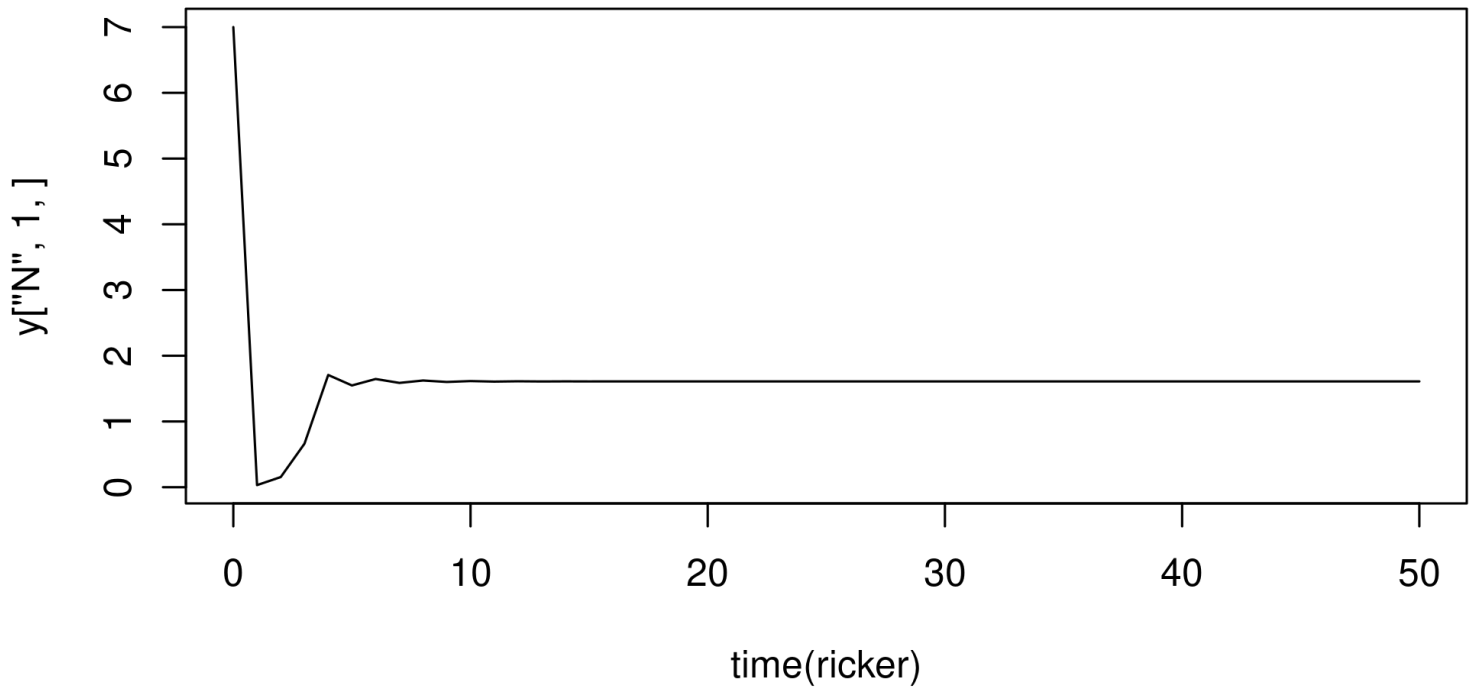
```
coef(ricker)
```

```
##         r     sigma       phi         c       N_0       e_0
## 44.70118   0.30000 10.00000   1.00000   7.00000   0.00000
```

- These are the parameters at which the simulations and deterministic trajectory computations above were done.
- We can run these at different parameters:

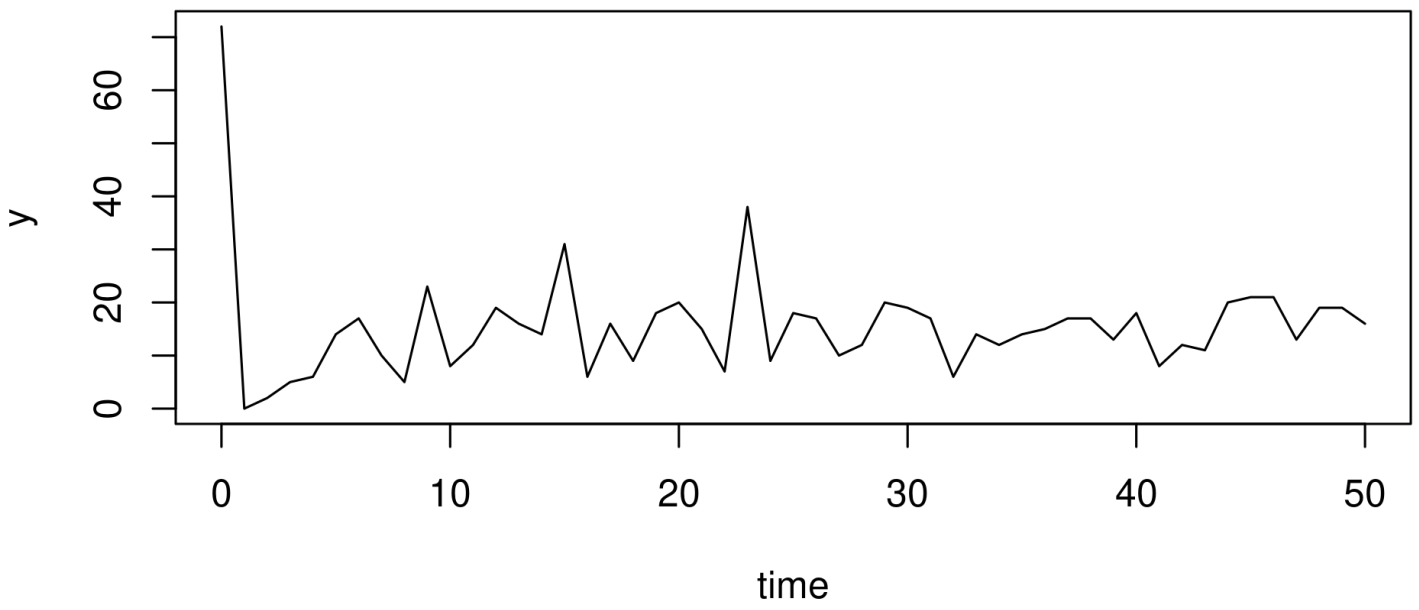
```
theta <- coef(ricker)
theta[c("r","N.0")] <- c(5,3)
y <- trajectory(ricker,params=theta)
plot(time(ricker),y["N",1,],type="l")
```

Working with model parameters II




```
x <- simulate(ricker,params=theta)
plot(x,var="y")
```

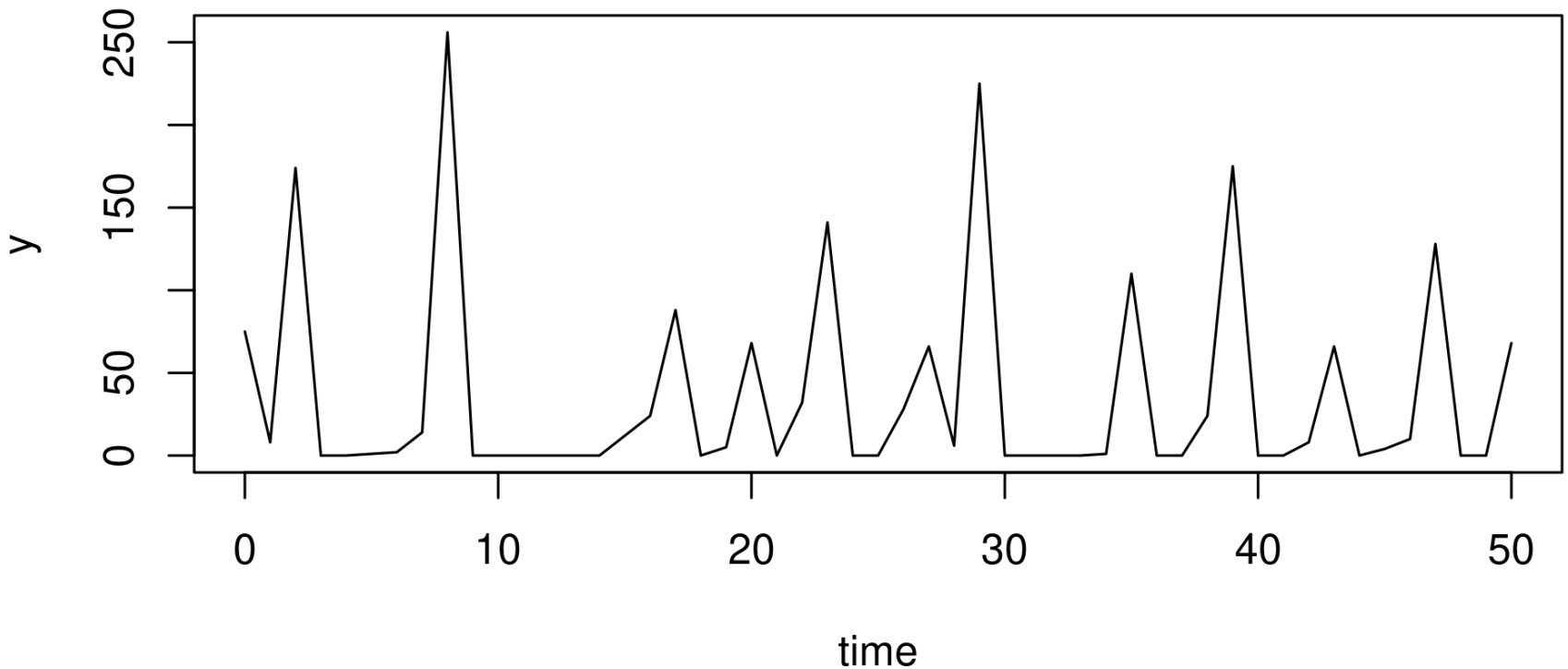
Working with model parameters III



- We can also change the parameters stored inside of `ricker`:

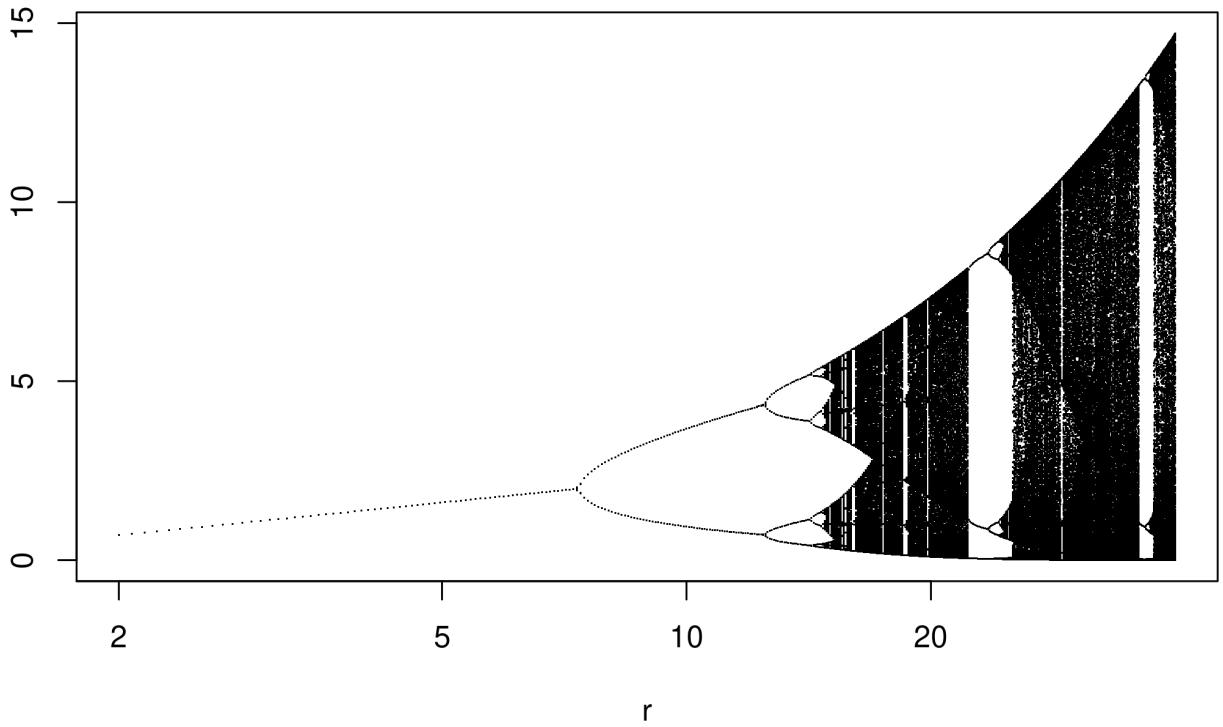
```
coef(ricker,c("r","N.0","sigma")) <- c(39,0.5,1)
coef(ricker)
plot(simulate(ricker),var="y")
```

```
##      r sigma   phi     c   N_0   e_0   N.0
##   39.0   1.0  10.0   1.0   7.0   0.0   0.5
```



It is possible to work with more than one set of parameters at a time:

```
p <- parmat(coef(ricker),500)
p["r",] <- seq(from=2,to=40,length=500)
y <- trajectory(ricker,params=p,times=200:1000)
matplot(p["r",],y["N",,],pch=".",col='black',xlab='r',ylab='N',log=
```



This is a bifurcation diagram (`https://en.wikipedia.org/wiki/Bifurcation_diagram`) for the Ricker equation.

Question 10.3. How do you interpret this bifurcation diagram?

- What does it mean when the single line for small values of r splits into a double line, around $r = 0.8$?

- What does it mean when solid vertical lines appear, around $r = 18$?

- A bifurcation diagram like this can only be computed for a deterministic map. However, the bifurcation diagram for the deterministic skeleton can be useful to help understand a stochastic process. We'll see an example later in this chapter.

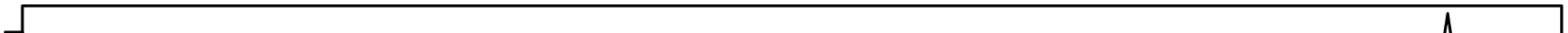
Burn-in

- Look at the R code for the bifurcation diagram. Notice that the first 200 iterations of the Ricker map are discarded, by setting `times=200:1000`. This is a technique called **burn-in**.
- This is used when aiming to simulate the steady state of a dynamic system, ignoring **transient behavior** from initial conditions.

Inference algorithms in pomp

- pomp provides a wide range of inference algorithms. We'll learn about these in detail soon, but for now, let's just look at some of their general features.
- The `pfilter` function runs a simple **particle filter**, which is a Monte Carlo algorithm that can be used to evaluate the likelihood at a particular set of parameters. One uses the `Np` argument to specify the number of particles to use:

```
pf <- pfilter(ricker,Np=1000)
class(pf)

## [1] "pfilterd_pomp"
## attr(,"package")
## [1] "pomp"

plot(pf)
```



Building a custom pomp object

A real pomp data analysis begins with constructing one or more pomp objects to hold the data and the model or models under consideration. We illustrate this process a dataset of the abundance of the great tit (*Parus major* in Wytham Wood, near Oxford (**?**).
First, we load and plot the data:

```
dat <- read.csv("parus.csv")
head(dat)

##   year pop
## 1 1960 148
## 2 1961 258
## 3 1962 185
## 4 1963 170
## 5 1964 267
## 6 1965 239

plot(pop~year,data=dat,type='o')
```

Let's suppose that we want to fit the stochastic Ricker model discussed above to these data.

- The call to construct a `pomp` object is, naturally enough, `pomp`.
- Documentation on this function can be had by doing `?pomp`.
- Do `class?pomp` to get documentation on the `pomp` class.
- Learn about the various things you can do once you have a `pomp` object by doing `methods?pomp` and following the links therein.
- Read an overview of the package as a whole with links to its main features by doing `package?pomp`.
- A complete index of the functions in `pomp` is returned by the command `library(help=pomp)`.
- The home page for the `pomp` project is (http://kingaa.github.io/pomp); there you have access to the complete source code, manuals, mailing lists, etc.

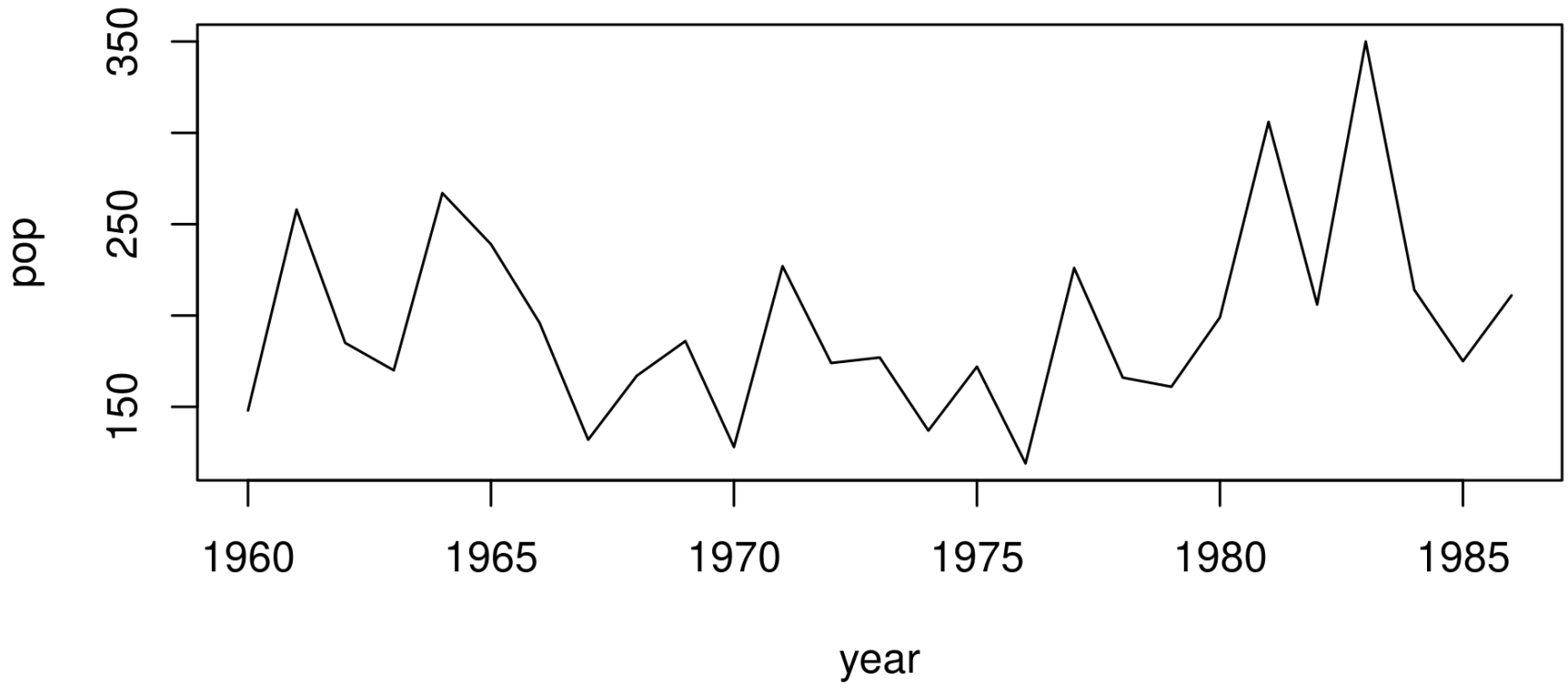
The simplest `pomp` object has only the data:

```
parus <- pomp(dat,times="year",t0=1959)
```

The `times` argument specifies that the column labelled "year" gives the measurement times; `t0` is the "zero-time", the time at which the state process will be initialized. We've set it to one year prior to the beginning of the data.

- We can now plot the data:

```
plot(parus)
```



Adding in the deterministic skeleton

We can add the Ricker model deterministic skeleton to the `parus` `pomp` object. Since the Ricker model is a discrete-time model, its skeleton is a map that takes P_n to P_{n+1} according to the Ricker model equation

$$P_{n+1} = r\,P_n\,\exp(-P_n).$$

We provide this to `pomp` in the form of a `Csnippet`, a little snippet of C code that performs the computation.

```
skel <- Csnippet("DN = r*N*exp(-N);")
```

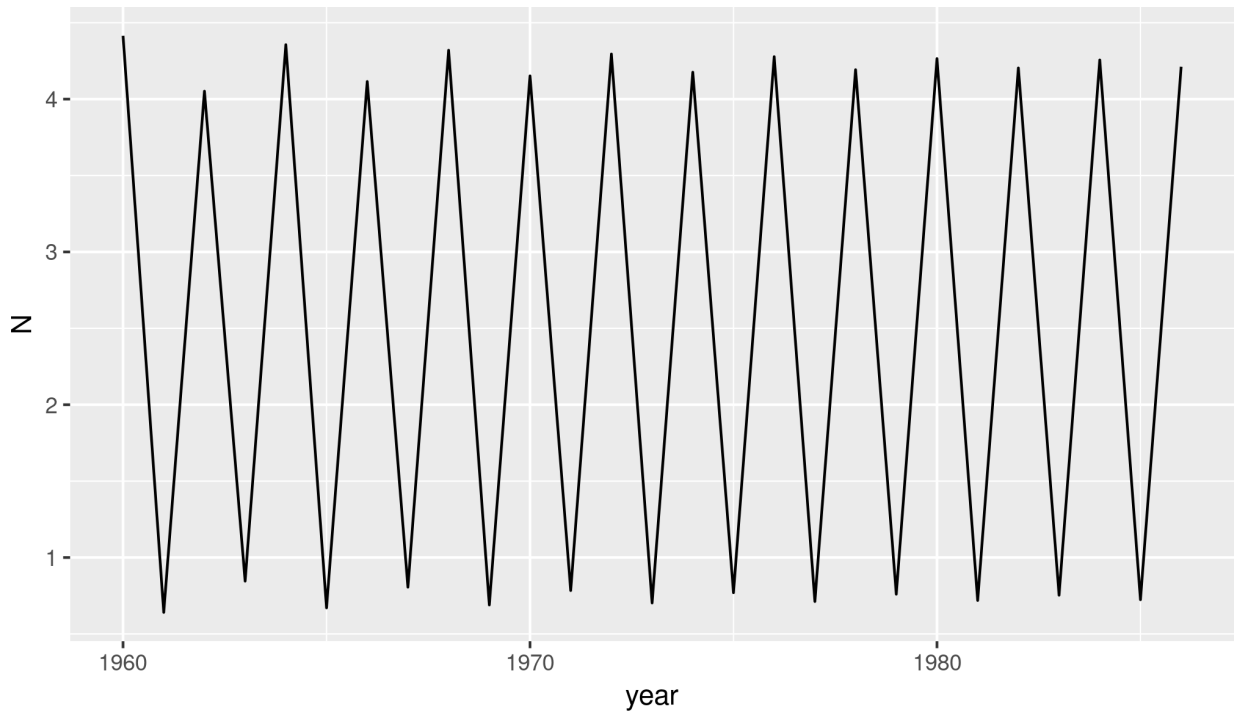
We then add this to the `pomp` object:

```
parus <- pomp(parus,skeleton=map(skel),statenames="N",paramnames="r"
```

Note that we have to inform `pomp` as to which of the variables we've referred to in `skel` is a state variable (`statenames`) and which is a parameter (`paramnames`).

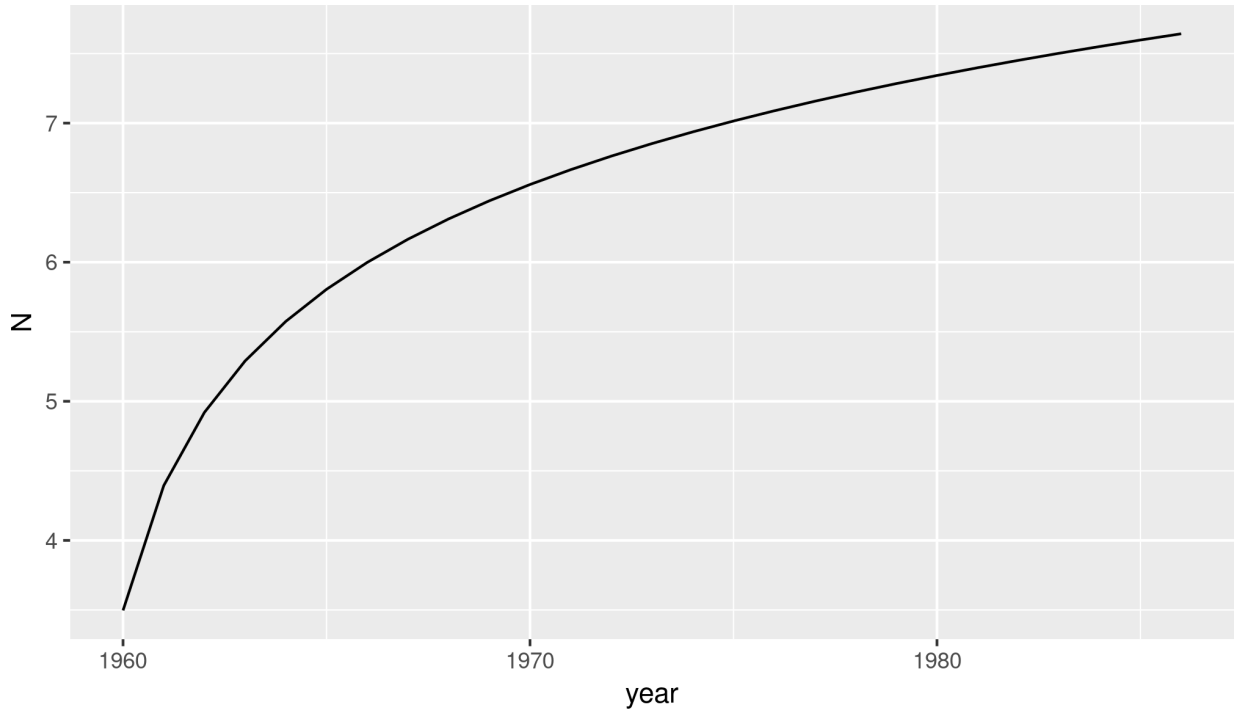
With just the skeleton defined, we are in a position to compute the trajectories of the deterministic skeleton at any point in parameter space. For example,

```
traj <- trajectory(parus,params=c(N.0=1,r=12), format="data.frame")
ggplot(data=traj,aes(x=year,y=N))+geom_line()
```



- Note that the dynamics become very different if the skeleton is considered as the derivative of a differential equation rather than as a discrete time map. It is harder to get chaotic dynamics in a continuous time system.

```
parus2 <- pomp(parus,skeleton=vectorfield(skel),statenames="N",para
traj2 <- trajectory(parus2,params=c(N.0=1,r=12),format="data.frame"
ggplot(data=traj2,aes(x=year,y=N))+geom_line()
```



A note on terminology

- If we know the state, $x(t_0)$, of the system at time t_0, it makes sense to speak about the entire trajectory of the system for all $t > t_0$.
- This is true whether we are thinking of the system as deterministic or stochastic.
- Of course, in the former case, the trajectory is uniquely determined by $x(t_0)$, while in the stochastic case, only the probability distribution of $x(t)$, $t > t_0$ is determined.
- In `pomp`, to avoid confusion, we use the term "trajectory" exclusively to refer to **trajectories of a deterministic process**. Thus, the `trajectory` command iterates or integrates the deterministic skeleton forward in time, returning the unique trajectory determined by the specified parameters. When we want to speak about sample paths of a stochastic process, we use the term **simulation**.
- Accordingly, the `simulate` command always returns individual sample paths from the POMP. In particular, we avoid "simulating a set of differential equations", preferring instead to speak of "integrating" the equations, or "computing trajectories".

Adding in the process model simulator

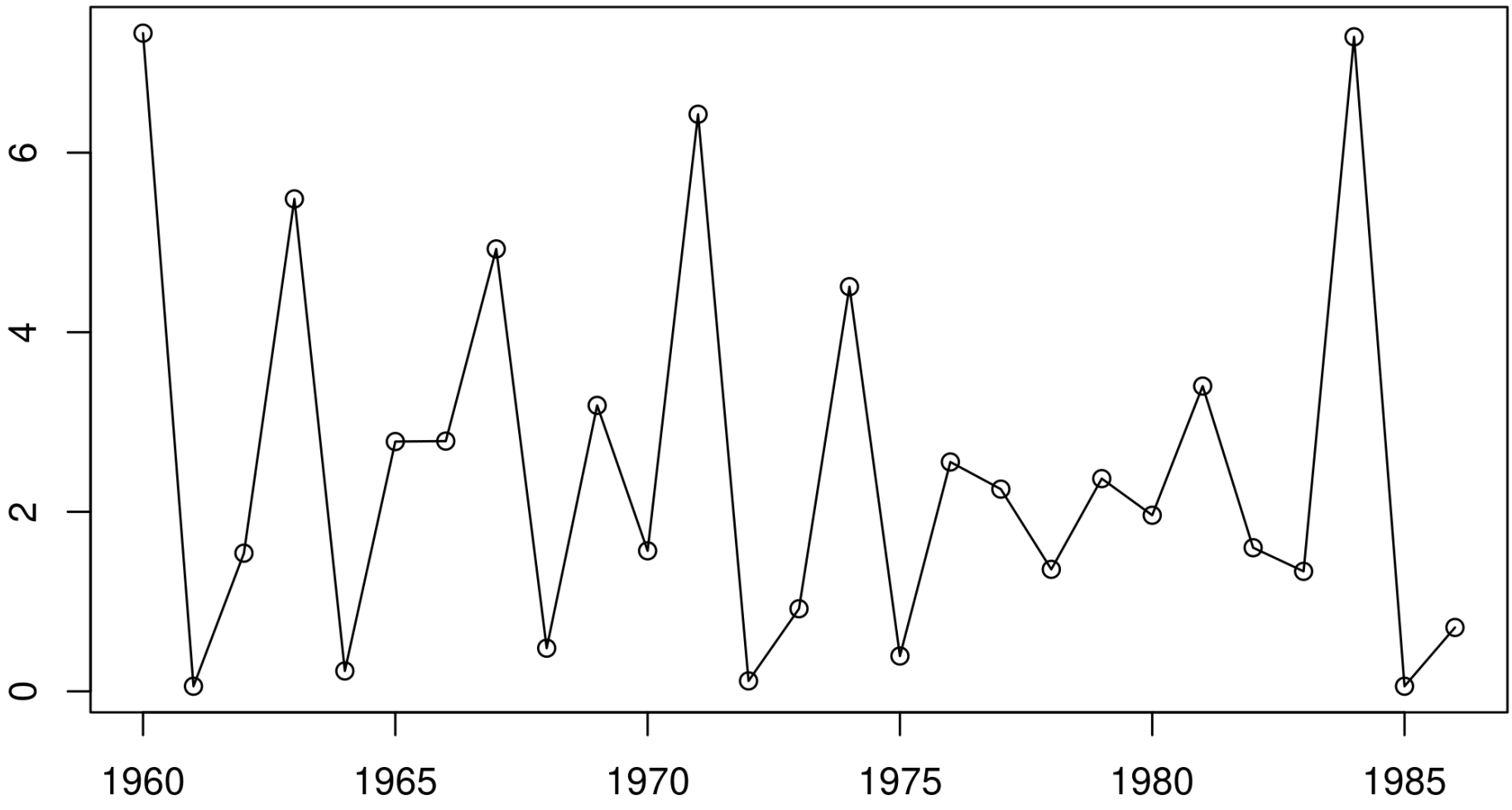
- We can add the stochastic Ricker model to `parus` by writing a Csnippet that simulates one realization of the stochastic process, from an arbitary time t to $t+1$, given arbitrary states and parameters:

```
stochStep <- Csnippet("
  e = rnorm(0,sigma);
  N = r*N*exp(-N+e);
")
pomp(parus,rprocess=discrete.time.sim(step.fun=stochStep,delta.t=1)
     paramnames=c("r","sigma"),statenames=c("N","e")) -> parus
```

- Note that in the above, we use the `exp` and `rnorm` functions from the C language API for R (`https://cran.r-project.org/doc/manuals/R-exts.html`)
- In general any C function provided by R is available to you. `pomp` also provides a number of C functions that are documented in the header file, `pomp.h`, that is installed with the package.
- See the `Csnippet` documentation (`?Csnippet`) to read more about how to write them.

- At this point, we have what we need to simulate the stochastic Ricker model.

```
sim <- simulate(parus,params=c(N.0=1,e.0=0,r=12,sigma=0.5),
                format="data.frame")
plot(N~year,data=sim,type='o')
```



Adding in the measurement model and parameters

- We complete the specification of the POMP by specifying the measurement model. To obtain the Poisson measurement model described above, we write two Csnippets. The first simulates:

```
rmeas <- Csnippet("pop = rpois(phi*N);")
```

- The second computes the likelihood of observing pop birds given a true density of N:

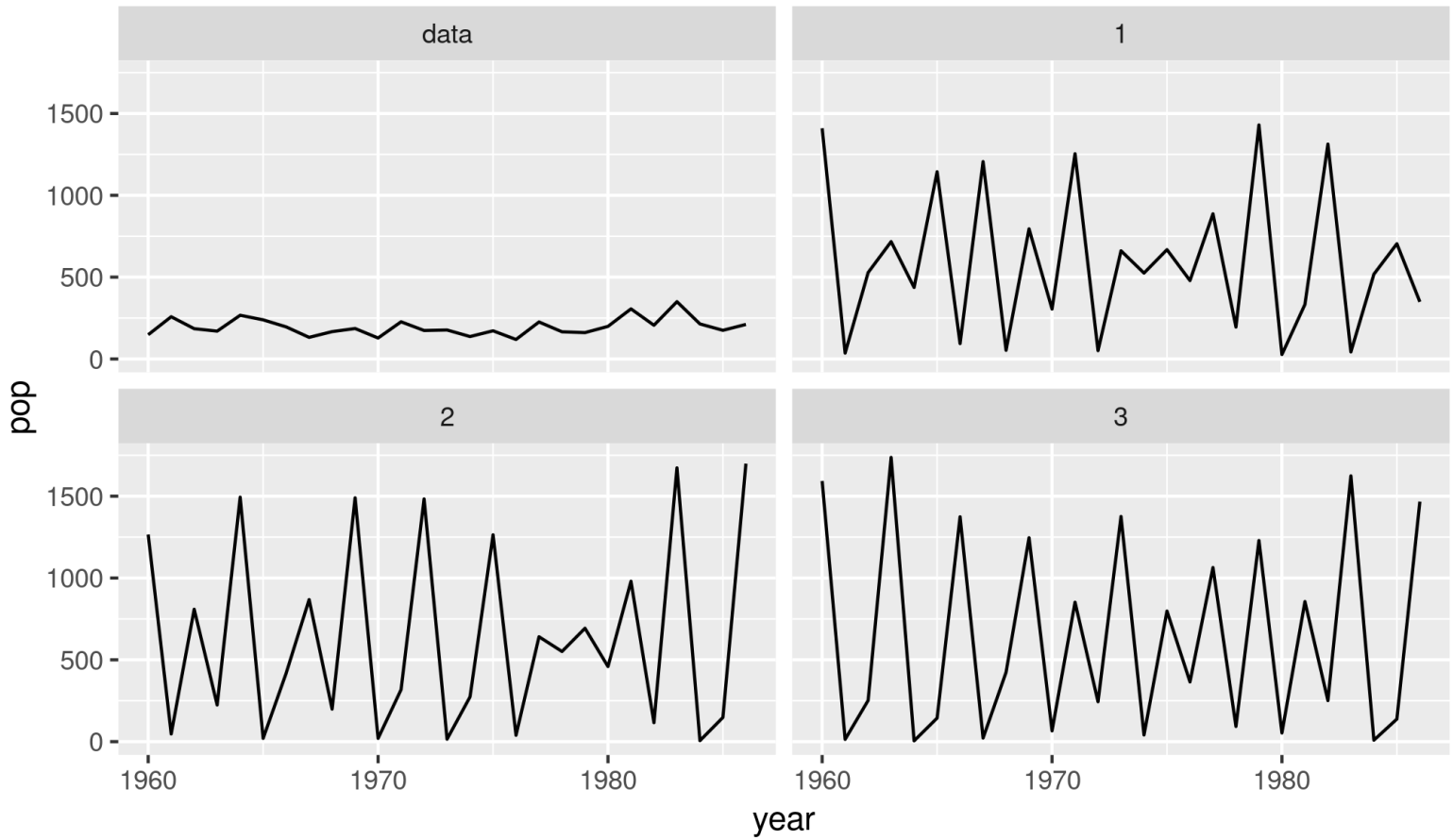
```
dmeas <- Csnippet("lik = dpois(pop,phi*N,give_log);")
```

- Note the give_log argument. When this code is evaluated, give_log will be set to 1 if the log likelihood is desired, and 0 else.
- We add these specifications of rmeasure and dmeasure into the pomp object:

```
pomp(parus,rmeasure=rmeas,dmeasure=dmeas,statenames=c("N"),
  paramnames=c("phi")) -> parus
```

- To simulate, we must add some parameters to the pomp object:

```
coef(parus) <- c(N.0=1,e.0=0,r=20,sigma=0.1,phi=200)
sims <- simulate(parus,nsim=3,format="data.frame",
  include.data=TRUE)
ggplot(data=sims,mapping=aes(x=year,y=pop))+geom_line()+
  facet_wrap(~.id)
```



Exercise: Ricker model parameters

- Fiddle with the parameters to try and make the simulations look more like the data.
- This will help you build some intuition for what the various parameters do.

Exercise: reformulating the Ricker model

- Reparameterize the Ricker model so that the scaling of P is explicit:

$$P_{n+1} = r\,P_n\,\exp\left(-\frac{P_n}{K}\right).$$

- Modify the `pomp` object we created above to reflect this reparameterization.
- Modify the measurement model so that

$$\mathrm{pop}_n \sim \mathrm{Negbin}(\phi\,P_n, k),$$

  i.e., pop_n is negative-binomially distributed with mean $\phi\,P_t$ and clumping parameter k.
- See `?NegBinomial` for documentation on the negative binomial distribution and the R Extensions Manual section on distribution functions (`https://cran.r-project.org/doc/manuals/R-exts.html`) for information on how to access these in C.

Exercise: The Beverton-Holt model

- Construct a `pomp` object for the *Parus major* data and the **stochastic Beverton-Holt** model,

$$P_{n+1} = \frac{a\,P_n}{1+b\,P_n}\,\varepsilon_n,$$

  where a and b are parameters and

$$\varepsilon_t \sim \text{Lognormal}(-\tfrac{1}{2}\sigma^2, \sigma^2).$$

- Assume the same measurement model as we used for the Ricker model.

Acknowledgments and License

- These notes build on previous versions at `ionides.github.io/531w16` and `ionides.github.io/531w18`.
- Those notes draw on material developed for a short course on Simulation-based Inference for Epidemiological Dynamics (`http://kingaa.github.io/sbied/`) by Aaron King and Edward Ionides, taught at the University of Washington Summer Institute in Statistics and Modeling in Infectious Diseases, from 2015 through 2018.
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