EEB 201: Introduction to R for Ecology and Evolutionary Biology

Introduction to dynamic modeling

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Learning objectives for my section

By the end of this section you will:

- Have a working knowledge of control statements in R
- Be able to write your own computer programs to simulate and plot population dynamics (in discrete time).
- Convert your simulation to a function, and write a program to perform sensitivity analysis.
- Have seen how to write your own computer programs to simulate and plot population dynamics in continuous time (ODE models)

Lightning review...

Programming in R

- Scripts are simply a collection of commands saved in a text file.
 - Make sure you use a non-formatted text editor, not a word processor!
 - Save the script in your working directory
 - Run the script using the source () command
- Functions are objects in R's workspace (just like variables)
 - We can define functions to do specific tasks.
 - Note: we need to get functions into R's workspace, by source-ing them once (or entering at the command line).

Flow control: conditional execution

- Sometimes we only want to execute part of our program under certain conditions.
- Use an **if statement**
 - express your condition as a logical expression

xx > 10 xx == 2 xx >= yy length(xx) != 0xx < 2 | xx > 20

 then you can set a block of code to be executed only if that condition is fulfilled

Flow control: conditional execution

Syntax in R

```
if (logical_expression) {
    expression_1
    ...
}
```

or for two options

```
if (logical_expression) {
    expression_1
    ...
} else {
    expression_2
    ...
}
```

Flow control: looping

- Often there will be tasks that you want to repeat many times.
- Can accomplish this using a **for loop** or a **while loop**.

for loops

- Use to repeat a fixed number of times.
- Define a vector with a set of values, and go through the loop once for each value.
- Often: use index variable, e.g. (ii in 1:10)

while loops

- Use to repeat until some condition isn't met anymore.
- Define the logical condition that needs to be satisfied.
- Repeat the loop until the condition is false.

Flow control: looping

```
<u>Syntax in R – for loops</u>
for (xx in 1:100) {
       expression 1
}
or more generally
for (xx in someVector)
       expression 1
       . . .
}
```

Syntax in R – while loops

```
while (logical_expression) {
    expression_1
    ...
}
```

Flow control: looping

<u>Example</u>

- Two ways of doing an operation 10 times
- Example: calculating compound interest on your bank balance for 10 years

With a for loop	With a while loop
money <- 100 interest <- 0.03	money <- 100 interest <- 0.03
<pre>for (tt in 1:10) { money <- money*(1+interest)</pre>	tt <- 1
}	while (tt <= 10) { money <- money*(1+interest) tt <- tt+1

}

Programming style

- Be clear rather than clever.
 - You'll be glad when you have to come back to a program you wrote two years ago.... to analyze new data or modify your analysis.
- Use meaningful variable names
 - birthRate and probSurvival instead of b and p
- When using simple variable names (x, y, i, j, etc), it's better to use double letters (xx, yy) since they're easier to find (and replace) using automated text search functions.

Programming style

- Comments! # you can never have too many
- Put a line or two of comments at the top of your program to say what it does.
 - Use 'sub-headings' to mark sections of code as well
- White space
 - leave blanks lines to separate blocks of code
 - use indentation consistently to indicate lines of code within loops or if statements
 - R doesn't insist on this like some languages, but it will help you keep your thinking straight, keep your parentheses matched up, and avoid bugs.

Pseudo-code

- **Pseudo-code** is an informal way to plan out the structure and logic of your programs.
- When pseudo-coding, DON'T worry about the syntax of the programming language you're using, but DO pay attention to the variables and flow control structures you will use.
- Because the basic structures of many high-level programming languages are the same, your pseudo-code will translate easily R, Matlab, python, or many other languages.

Pseudo-code example

Goal: Determine how many students pass the bootcamp.

set the number of passes to zero# set the number of fails to zero

loop over the number of students in the class

- # if the student completed their exercises from day 1
 - # add one to the number of passes
- # or else if they didn't complete their exercises
 - # add one to the number of fails
 - # print "Come on, this is the first thing we've asked you do in grad school!"

show the result

Exercise break: Pseudo-code

The **geometric growth model** is the simplest model for population growth in discrete time. It assumes that every year the size of the population changes by the same factor, *R*.

 $N(t+1) = R \times N(t)$

Exercise: write pseudo-code for a program that simulates the growth of a population for 10 years, starting with N=100 animals and assuming R = 1.05, and prints the final population size.

Bonus: modify the pseudo-code so the program will make a plot of *N* versus *t*.

Terminology: Ingredients of a dynamic model

State variables: quantities that describe the entities of interest for your model.

e.g. population size, disease prevalence

Parameters: quantities that govern the dynamics, but don't describe the state of the system and (typically) don't change over time.

e.g. per capita birth rate, carrying capacity, transmission rate

Dynamic equations: a set of equations or rules specifying how state variables change over time, as a function of current and past values of the state variables.

General layout of modeling scripts

- 1. Setup statements, if needed (e.g. loading packages)
- 2. Input data, set parameter values, and/or set initial conditions
- 3. Perform the calculations
- 4. Display the results by plotting, saving, or showing on-screen.

One useful habit is to lay out the program in pseudocode, then use the pseudocode as commented headings in your real code.

Exercise break: your first model

- 1. Modify the pseudocode for your geometric growth model, using this general layout as a template.
 - 1. Setup statements, if needed (e.g. loading packages)
 - 2. Input data, set parameter values, and/or set initial conditions
 - 3. Perform the calculations
 - 4. Display the results by plotting, saving, or showing on-screen.
- Fill this in with actual R code, so you have a program that simulates the geometric growth model for given initial value (N0) and R, and plots the result.

A program for the geometric model

geometricGrowthScript.R

a script to simulate and plot the discrete logistic model

Setup

Set initial conditions and parameter values

initialize variable to a vector of NA values

use a loop to iterate the model the desired number of times

plot the results

Exercise break: your first model

- Fill this in with actual R code, so you have a program that simulates the geometric growth model for given initial value (N0) and R, and plots the result.
 - Save this script, with an appropriate name. Your first modeling script!
- 3. Modify this program to simulate the discrete logistic growth model, which is defined by this equation:

$$N(t+1) = N(t) \left(1 + r_d \left(1 - \frac{N(t)}{K} \right) \right)$$

What do you need to change in the code? (how many lines will change?)

4. Play around with your model. Use different parameter values of N0 and R, to figure out the conditions where your population will approach carrying capacity, shrink to zero, or do something else.

So that was fun.

But also kind of annoying.

Wouldn't it be nice if there was an efficient way to re-run your program with different parameter values?

Programming your own functions

Writing your own functions is the most powerful way to make R work flexibly and efficiently for you.

→ User-defined functions enable you to reduce long stretches of complicated programming to a single command.

A function takes in arguments, performs some operations, and returns a value.

To define a function, you need to

- choose a name for the function (avoid reserved words)
- define the arguments that need to be passed to the function
- define the operations
- set what value the function returns

Programming your own functions

<u>R syntax</u>

```
name <- function(argument_1, argument_2, ...) {
    expression_1
    expression_2
    ...
    return(output)
}</pre>
```

Example: program to build a three-digit number

```
> numberify <- function(xx, yy, zz) {
+     myNumber <- xx * 100 + yy * 10 + zz
+     return(myNumber)
+ }</pre>
```

Inputs: default values for arguments

You can assign default values to function arguments by giving them a value in the function definition.

```
> numberify <- function(xx=1, yy=1, zz=1) {
+     myNumber <- xx * 100 + yy * 10 + zz
+     return(myNumber)
+ }</pre>
```

Any argument with a default value is optional when you call the function. If you pass fewer values than the function has arguments, then R will assign them from left to right, unless you name the arguments as you pass values.

```
> numberify() > numberify(3)
```

> numberify(3,2) > numberify(yy=3)

The function workspace and variable scope

- When a function is executed, R sets aside memory for a separate workspace for the function to operate.
- The function can define new variables and conduct all its operations in complete isolation from the main workspace.
- When the operations are complete, the function returns the appropriate quantity and all other information in the function workspace is **lost**.
 - → If you want to use something outside the function, you need to return it!

Stopping and outputs

The function will continue evaluating until:

- it hits the first return() statement, after which it returns the requested value and quits.
 - note that there can be multiple return() statements in a function, e.g. in a branching program structure
- it runs out of commands to run, without hitting a return() statement.
 - sometimes the returned value isn't the point of the function, e.g. in a function whose purpose is to make a plot.
 - In this case, if you try to assign the function output to a variable, it returns the value of the last expression it evaluated (even if NULL).

If you want something returned, code it explicitly with return().

Return to logistic model

How can we program the discrete logistic model as a function?

- what do we want it to do?
- what arguments do we want to pass to it?
- what outputs do we want?

(Pseudo)code for a model function is very similar to a script, except many of the parameter values and initial conditions are often passed as arguments to the function, where they were set 'manually' in the script.

Example: converting a model script to a function

By converting a script to a function, you can make it quick and easy to run the model with different parameter values or initial conditions.

The conversion process is easy – <u>for example</u>:

```
# Simple model script
                                             # Function version
# Define parameter values and ICs
RR <- 1.05
                       Basic change: just
                                            geomFun <- function(RR, N0, ttMax){</pre>
                       moved parameters,
NO < -100
                                                 # Initialize vector to hold output
                      ICs from body of script
ttMax <- 10
                                                 NN <- rep(NA,ttMax+1)</pre>
                      to function arguments
                                                 NN[1] < - N0
# Initialize vector to hold output
NN <- rep(NA,ttMax+1)</pre>
                                                 # Use a for loop to step forward
                                                 for (tt in 1:ttMax) {
NN[1] < - NO
                                                      NN[tt+1] <- RR*NN[tt]
# Use a for loop to step forward
for (tt in 1:ttMax) {
    NN[tt+1] <- RR*NN[tt]</pre>
                                                 plot(1:(ttMax+1),NN,lty=2,type=`l',
                                                      ... xlab='t', ylab='Population
                                                      size')
plot(1:(ttMax+1),NN,lty=2,type=`l',...
                                            }
    xlab=`t', ylab=`Population size')
```

Example: converting a model script to a function

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The conversion process is easy – <u>for example</u>:

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NO < -100
                                                 # Initialize vector to hold output
                      ICs from body of script
ttMax <- 10
                                                 NN <- rep(NA,ttMax+1)</pre>
                      to function arguments
                                                 NN[1] < - N0
# Initialize vector to hold output
NN <- rep(NA,ttMax+1)</pre>
                                                 # Use a for loop to step forward
                                                 for (tt in 1:ttMax) {
NN[1] < - NO
                                                      NN[tt+1] <- RR*NN[tt]
# Use a for loop to step forward
for (tt in 1:ttMax) {
    NN[tt+1] <- RR*NN[tt]</pre>
                                                 plot(1:(ttMax+1),NN,lty=2,type=`l',
                                                      ... xlab='t', ylab='Population
                                                      size')
plot(1:(ttMax+1),NN,lty=2,type=`l',...
                                                 return(NN)
    xlab=`t', ylab='Population size')
                                            }
```

Example: converting a model script to a function

Now you can run the full model, for any parameter values and initial conditions, using a single statement (by *calling* the function).

```
> geomFun(RR=1.01, N0=200, ttMax=20)
```

```
> myOutput <- geomFun(RR=1.01, N0=200, ttMax=20)</pre>
```

Exercise break

Convert your discrete logistic model into a function.

Use this function to explore the model's dynamics with ease and grace.

Exploring your model systematically:

sensitivity analysis

Now you can run your whole model in a single line.

You're in a position to do fancier things, such as running the model many times to analyze the sensitivity to different parameter values.

Pseudocode for a sensitivity analysis

Define parameter values; use a vector to hold a range of values for the parameter(s) you wish to vary.

Initialize a matrix to collect all outputs

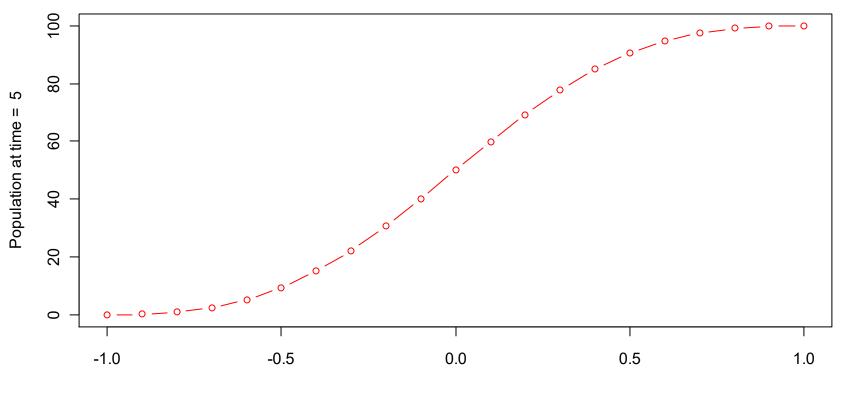
- # Use a **for loop** to repeatedly run the model and collect output
 - # NOTE: this for loop is **NOT** over the timesteps of the model, it is over the set
 - # of different parameter values for which you want to run the model.
 - # Use your function to run the model in a single line within the loop.

analyze results

Sensitivity analysis: response to parameter values

How does the population size in 5 years depend on growth rate r_d ?

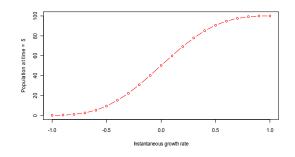
(initial conditions and other parameter values held constant)



Sensitivity to value of r_d

growth rate r_d

To make a plot of model summary output versus parameter value



Define parameter values

for parameter of interest, make a vector of values you want to consider

Initialize vector to hold summary values

Use a **for loop** to repeatedly run the model and plot output

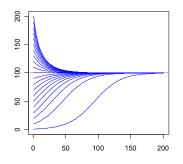
- # You are looping over the list of values you want to use for the
- # parameter you're varying.
- # Each time through loop, run the model with the current parameter
- # values and store the summary values in the ith element of your
- # results vector

Plot the results vector versus the vector of parameter values.

A script for sensitivity analysis

```
# Sensitivity analysis of discrete logistic model
# plot population size at t=5 for range of rd values
# set parameter values
ttCollect < - 5
NO <- 50
KK <- 100
rdVec <- seq(-0.5, 0.5, by=0.1) # vector of values for key parameter
# initialize vector with null values
nnVec <- rep(NA, 1, length(rdVec))</pre>
# loop over values of key parameter, and run model for each value
for (ii in 1:length(rdVec)) {
       logisticOutput <- discreteLogisticFun(N0, rd=rdVec[ii], KK,</pre>
               PLOTFLAG=0)
       nnVec[ii] <- logisticOutput[ttCollect]</pre>
}
# plot the results
plot(rdVec, nnVec, xlab='Instantaneous growth rate, r d',
        ylab=paste('Population at time = ',as.character(ttCollect)),
       type='b', col='red', main='Sensitivity to value of r d')
```

To plot many overlaying curves



Define parameter values

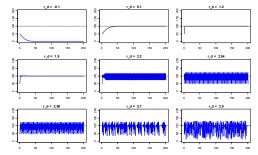
for parameter of interest, make a vector of values you want to consider

Initialize empty plot window to catch all the resulting plots
plot(0, type='n',... etc)

Use a **for loop** to repeatedly run the model and plot output

- # You are looping over the list of values you want to use for the
- # parameter you're varying.
- # Each time through loop, run the model with the current parameter
- # values and plot the results using lines()

To make many plots in different sub-windows



Define parameter values

for parameter of interest, make a vector of values you want to consider

Initialize plot window to have right number of rows and columns
par(mfrow=c(3,3))

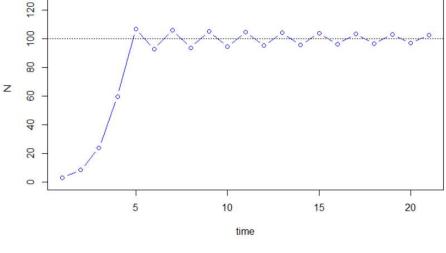
Use a **for loop** to repeatedly run the model and plot output

- # You are looping over the list of values you want to use for the
- # parameter you're varying.
- # Each time through loop, run the model with the current parameter
- # values and plot the results using plot()

Discrete-time models

N(t+1) = R N(t)

Difference equations, maps



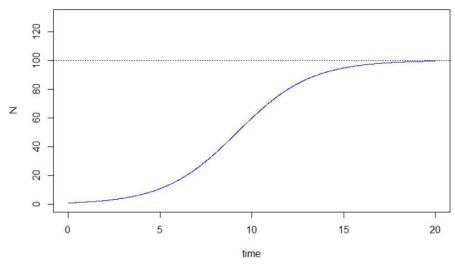
<u>Strengths</u>

- Seasonal systems
- Discretized data
- Easy coding!

Continuous-time models

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

ODEs (ordinary differential eqs)



<u>Strengths</u>

- Non-seasonal systems
- Events occur at any time
- Easier math analysis

Simulating an ODE model in R

- install package 'deSolve'
- load the package into memory using library(deSolve)

We will use a function called Isoda that is a versatile and robust numerical integrator for ordinary differential equations.

 powerful tool but you need to interact with it in a very specific way – be careful with syntax!

Syntax for lsoda

Generic syntax for lsoda is: output <- lsoda(init, tseq, ODEfunction, pars) where:

init is the initial value of the state variable
tseq is a vector of the time points where the model will be evaluated
ODEfunction is a place-holder for the name of the function holding the
model equations

pars is a vector containing any parameters used in the model

output is the variable where lsoda will return its results.

Syntax for lsoda

The function holding the model equations must have syntax:

```
ODEfunction <- function(tt, yy, pars) {
    derivs <- [insert model equations]
    return(list(derivs))
}</pre>
```

where:

```
tt is a variable used by R to keep track of the timestep
yy is the state variable (or vector of state variables, for multi-variate
models)
```

```
pars is your vector of model parameters
```

derivs is an internal variable that records the time series of results

1soda example: exponential growth

$$\frac{dN}{dt} = rN$$

```
expGrowthODE <- function(tt, NN, pars) {</pre>
   derivs <- pars['rr'] * NN</pre>
    return(list(derivs))
}
init <- 1
                                          Note new way of indexing a vector.
tseq < - seq(0, 20, by=0.01)
                                          Access with pars['rr']
pars <- c(rr = 0.1) \leftarrow
                                          Don't need to use this method, but
                                          it's useful when you have lots of
                                          parameters.
Then call with:
```

expOutput <- lsoda(init, tseq, expGrowthODE, pars)</pre>

Output from lsoda

The output from our command:

expOutput <- lsoda(init, tseq, expGrowthODE, pars)</pre>

will be a matrix made up of two column vectors.

The first column will be the time points where the state of the system is recorded, and the second column will be the corresponding values of the state variable.

```
> expOutput
    time 1
[1,] 0.00 1.000000
[2,] 0.01 1.001001
[3,] 0.02 1.002002
[4,] 0.03 1.003005
...
```

So we can plot the dynamics with:

plot(expOutput[,1], expOutput[,2], col='blue', type='l')

Exercise: modify code to model logistic growth

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

```
logisticGrowthODE <- function(tt, NN, pars) {
    derivs <- pars['rr'] * NN * (1 - NN/pars['KK'])
    return(list(derivs))
}
init <- 1
tseq <- seq(0, 20, by=0.01)
pars <- c(rr = 0.1, KK = 100)</pre>
```

Then call with:

logOutput <- lsoda(init, tseq, logisticGrowthODE, pars)</pre>