ECL/PBG 233: Computational methods in population biology (Marissa Baskett and Sebastian Schreiber) Programming info sheet

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Rules of coding

- 1. Any time you write a line of code more than once, program it as a function so you only have one place where you need to look for any corrections or changes.
- 2. Break your code down to individual functions that each preform an individual task so you can debug and test piece by piece ("functional decomposition").
- 3. Plan out your code beforehand, writing a phrase or sentence for each general step you plan to take (these might be your functions), then breaking those into smaller steps, until each is something you can turn into a line of code ("pseudocoding"); this is analogous to outlining a paper before writing full sentences to make sure you have logical flow and all of the pieces fit together.
- 4. Comment while you code so it's easier to remember what the code means when revisiting it.
- 5. Define parameters up front rather than using numbers within coded calculations so it's easy to find and change them.
- 6. Write your code as a script instead of at the prompt so it's easier to edit, save what worked, and run it again another day.
- 7. Specific to R (and Matlab): any time you can use vectors or matrices instead of for loops, try it; it's usually much faster.
- 8. Debugging:
 - (a) Test your functions for parameters/cases where you know the answer before running it for a more complicated case so you can make sure they work ("testing").
 - (b) When you can't figure out a bug, go line-by-line through the function, checking that you're getting what you expect from each command ("desk-checking"; R functions: debug, browser); you can also comment out lines to help you isolate a bug (in R, text after a #).
 - (c) Especially for code where others might be using your functions, build in warning and error messages for inappropriate values that might accidentally be passed (R functions: warning, stop; e.g., cases where zero or negative parameter values will give invalid results).

For more on best practices of coding, see:

- http://swcarpentry.github.io/slideshows/best-practices/index.html#slide-0
- http://journals.plos.org/plosbiology/article?id=10.1371/journal.pbio.1001745

Commands in R

Basics	
help (functionName)	Get quick help on function functionName; you can also use the
	Help menu
+ - * / ^	Simple addition, subtraction, multiplication, division, and power;
	element-by-element if you're using vectors or matrices
x = 4	Assign the value 4 to x
sin(x), cos(x), tan(x)	sine, cosine, and tangent
exp(x), log(x), log10(x)	exponential, natural log, base-10 log
abs(x), sqrt(x)	Absolute value, square root
$\mathbf{Re}(x), \mathbf{Im}(x)$	Real and imaginary parts of x
round(x), floor(x), ceiling(x)	Rounded value, floor (drop everything after the decimal), or ceil-
	ing (opposite of floor, round up anything with a decimal to the
	next largest integer) of x
rm (x)	clear the value stored in x ; $\mathbf{rm}(\text{list=ls}())$ clears all values

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Plotting	
plot (x, y, type="l", xlab="X	Plot y vs. x with a line (type l , could also be p for points, b
label", ylab="Y label",	for both, etc.) in color color (e.g., red, blue, etc.), with x-label
col="color", main="Title")	X label, y-label Y label, and title $Title$; all specifications but x
	and y are optional; if you want to put parameter values into any
	labeling, use the paste command
$ \mathbf{lines}(x, y,), \mathbf{points}(x, y,)$	Plot lines or points on an existing plot; note that you have to start
	the plot with plot (can be a blank line with type="n") and then
	use these; use the legend command to add a legend if desired
$\mathbf{matplot}(X, Y,)$	Plot the columns of matrix X against the columns of matrix Y
barplot (vals, beside=TRUE,	Bar plot of <i>vals</i> where bars are next to each other (beside=TRUE,
names.arg=labs,)	instead of stacked) with labels <i>labs</i> for the bars
$\mathbf{hist}(\mathbf{x},\mathbf{breaks}=20,\ldots)$	Histogram plot of \mathbf{x} with data broken in the specified number of
	equally space intervals (e.g. 20)
contour(x,y,z,nlevels = 10)	Contour plot with nlevels contours of the matrix z where x and y
	are the locations the grid lines where the z values were computed.
	To get filled contours, use filled.contour . Alternative contour
	plot commands are available in the lattice package.
image(z)	Color map plot based on values of z .
$\mathbf{pdf}(\text{file}=\text{"fileName.pdf"})$	Create file <i>fileName.pdf</i> to save plot in. Use this command before
	creating the plot.
dev.off()	Shut down current plot. For creating pdfs, you need to shut down
	the current plot before it saves the image as a pdf file.
$\mathbf{par}(\mathbf{mfrow} = \mathbf{c}(\mathbf{m}, \mathbf{n}), \mathbf{cex.axis} = \mathbf{q},$	This command can be used to control the way things are being
)	formatted in plots, e.g. the mfrow option creates a layoff of m by
	n subplots that get filled as further plot commands are executed,
	the cex.axis magnifies the axes by a factor of q , etc.

Vectors	
c (a, b, c)	A vector with values $a, b,$ and c (can be any number of values)
x = c(a=1, b=2, c=3)	A vector with values 1, 2, and 3 labeled as a , b , and c
startVal:endVal	A vector from $startVal$ to $endVal$ in increments of 1
rep(val, rep)	A vector of value val repeated rep times
seq(startVal, endVal, by=inc)	A vector from $startVal$ to $endVal$ in increments of inc
seq(startVal, endVal, length=nVals)	A vector from $startVal$ to $endVal$ of length $nVals$
v[n]	n^{th} element of vector v
length(v)	Length of vector v
$\mathbf{sum}(v)$	Sum of all entries in vector v (also works for matrices)
$\mathbf{cumsum}(v)$	Cumulative sum of vector v at each entry (e.g., if $v =$
	(a_1, a_2, a_3) , cumsum $(v) = (a_1, a_1 + a_2, a_1 + a_2 + a_3)$
min(v), max(v), range(v)	Minimum value, maximum value, or range of values in vector
	v (also works for matrices)
$\mathbf{mean}(v), \mathbf{var}(v), \mathbf{sd}(v)$	Mean, variance, and (sample) standard deviation of vector v
$\mathbf{cor}(v,w)$	Correlation of vectors v and w
$\mathbf{which}(v==val)$	Which entries of v equal value val (also works for matri-
	ces and can also use the other logical operators listed in the
	"Loops" table)
which.max(v)	Which entries of v equal the maximum value
$\mathbf{rev}(\mathbf{v})$	Reverse of vector v
$\mathbf{as.data.frame}(\mathbf{x})$	Turn object x into a data frame

Matrices	
matrix(v, Nrows, Ncols)	Create a matrix filled with entires v (a number, which will be put
	into all entries, or a vector of values) with Nrows rows and Ncols
	columns
$\mathbf{diag}(\mathbf{v},\mathbf{n})$	$n \times n$ matrix with v on the diagonal and zeros everywhere else
cbind (v1, v2,)	Combine vectors (or matrices) $v1, v2, \dots$ along columns
rbind (v1, v2,)	Combine vectors (or matrices) $v1, v2, \dots$ along rows
$ $ $\mathbf{nrow}(M), \mathbf{ncol}(M), \mathbf{dim}(M)$	Dimensions of matrix M (number of rows, number of columns, both
	dimensions in a vector of [nrow, ncol])
M[m,n], M[m,], M[,n]	For matrix M , entry in row m and column n , m^{th} row, or n^{th} column
$\mathbf{t}(\mathrm{M})$	Transpose of M
$\det(M)$	Determinant of M
ev = eigen(M)	Eigenvalues (evvalues$) and eigenvectors (evvectors$) of M
M%*%N	Matrix multiplication of M and N
M%x%N	Kronecker product of M and N (equivalently, kronecker (M, N))
M%o%N	Outer product of M and N (equivalently, outer (M, N))
rowSums(M), colSums(M)	Sum across rows or columns $(\mathbf{sum}(M) \text{ sums all entries})$

Scripts and functions	
# text	Comment (text is not read by R)
source("scriptName.R")	Run scriptName.R
$fnName = function(inputs) \{\}$	Define function fnName with inputs inputs
return(x)	Return value x at the end of a function
return(list(x,y))	Return multiple values at the end of a function
print (input)	Display <i>input</i> (a variable for its value or text in quotes) to
	the screen
out = optimize (fn, c(searchMin, search-	Find the minimum (out\$minimum) of function fn over the
Max))	range from searchMin to searchMax
$out = \mathbf{optim}(x0, fn)$	Find the minimum $(out\$par)$ of function fn given initial guess $x0$
debug(fn)	Debug function fn : lets you step through the function so you
	can examine it for debugging (hit return to go step by step, c
	to continue, or Q to quit; browser and traceback are useful
	debugging functions as well)
system.time(command)	Returns the amount of time required to execute <i>command</i> .
	Useful for estimating completion times for large simulations.

Loops	
for (x in 1:xf) {}	For each value of x from 1 to xf preform set of commands
$\mathbf{while}(\mathbf{cond})\{\}$	While the conditions <i>cond</i> are true, preform set of commands
$if(cond)\{\}else\{\}$	If the conditions <i>cond</i> are true, preform set of commands, and if not, preform
	another set of commands (following <i>else</i> , this part is optional); note that if
	you have a series of if/else statements, switch might work better
>,<,>=,<=,==	Tests for greater/less than, greater/less than or equal to, and equal to (e.g.,
	$x \le y$ returns TRUE if x is less than or equal to y and FALSE if not)
!, &,	Not, and, or (e.g., $x < y \& x < z$ returns TRUE if x is less than both y and
	z and FALSE otherwise)
lapply(v, fn)	Apply function fn to each element of vector v , returning a list; sapply
	preforms the same operation but returns a vector (or matrix), and both of
	these are options for avoiding time-consuming for loops

Numerical integration	
library(deSolve)	Load the library for numerical integration, must come before
	using lsoda
lsoda(n0, seq(t0,tf,dt), odeFun,	Numerically integrate the function odeFun given parameters
parms)	parms starting with values $n0$ over time vector $seq(t0,tf,dt)$.
	Final output is a data array. To get final output to be simply
	a matrix use ode instead of lsoda .
odeFun = function(t, n, parms)	Appropriate structure for a function for use in Isoda: order
$\{$ with(as.list(parms), $\{$ dn = re-	of inputs is $t, n, parms$, need to extract any input parameter
$\mathbf{turn}(\mathbf{list}(\mathbf{dn}))\})\}$	values out of list $parms$ using $with(as.list(parms), {})$, and
	need to return dn as a list

Random numbers	
rnorm(num, mean=m, sd=s)	num random normal variables from a distribution with mean m
	and standard deviation s . To compute uniform random num-
	bers use runif , Poisson distributed numbers rpoiss , exponen-
	tially distributed numbers rexp , binomially distributed numbers
	rbinom, etc.
dnorm (num, mean=m, sd=s)	Computes the density at <i>num</i> for a normal distribution with
	mean m and standard deviation s . To compute densities for uni-
	form random numbers use dunif , Poisson distributed numbers
	\mathbf{dpoiss} , exponentially distributed numbers \mathbf{dexp} , binomially dis-
	tributed numbers dbinom , etc.
pnorm (num, mean=m, sd=s)	Computes the distribution function at num for a normal distribu-
	tion with mean m and standard deviation s . To compute densi-
	ties for uniform random numbers use punif , Poisson distributed
	numbers ppoiss , exponentially distributed numbers pexp , bino-
	mially distributed numbers pbinom , etc.
$\mathbf{set.seed}(\mathbf{seed})$	Sets the "seed" of the random number generator to seed (a nat-
	ural number). Allows one to get replicatable results.
sample(v, num, replace=FALSE)	Sample num entries from the vector v without replacement (or
	replace=TRUE for with replacement)

Generalized Linear Models	
glm (formula, family, data)	formula is a linear formula of the form y $x1+x2++xk$ where
	y,x1,,xk are the names of data in the data frame entered into the
	data field. family corresponds to the statistical family being used
	for the fits. These families include binomial for logistic regressions
	on 0, 1 data (e.g. survival), gaussian for normally distributed er-
	rors around the linear trend (i.e. classical linear regression), poisson
	for counting data. Associated with each of these families is a "link"
	function that is used to transform the data e.g. the link function for
	the Poisson family is the log function.
summary(model)	Provides the summary statistics associated with the output of most
	statistical packages in R. model is the name of the output from a
	statistical model e.g. glm
<pre>predict(model,newdata,type)</pre>	provides predicted values from the statistical model <i>model</i> . The pre-
	dictor values (e.g. x1,x2,,xk) need to be supplied as a data frame in
	newdata. type determines the format of the output. The default is on
	the linear scale of the potentially transformed response variable. "re-
	sponse" provides the values on scale of the response variable (usually
	what one wants).

Data input/output	
save(x, file="data.Rdata")	Save x (can put in multiple objects, e.g., $\mathbf{save}(x,y,)$) as R
	data in data.Rdata
load("data.Rdata")	Load R data in file data.Rdata
x = scan(file = "data.txt")	Input data in data.txt file into a vector or list
A=read.table("data.txt")	Input data in data.txt file into a data frame; apply as.matrix
	to convert to a matrix
$\mathbf{write}(t(A), file="data.txt", ncol-$	Output matrix A to $data.txt$ file; use write.table for data
umn=dim(A)[2])	frames

Useful packages	
ggplot2	Improved and (more intuitively) flexible plot formatting
deSolve	ODE integration
FME	Includes sensitivity analyses for continuous-time models
mnormt	Multivariate normals
multicore	Parallel processing
knitr	Generating reports that integrate R code with text