ECL 298: Computational methods in population biology (Marissa Baskett and Sebastian Schreiber) Programming info sheet March 8, 2013

## 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 accidently be passed (R functions: warning, stop; e.g., cases where zero or negative parameter values will give invalid results).

## Commands in R

Basics	
help(functionName)	Get quick help on function <i>functionName</i> ; 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
$\mathbf{Re}(\mathbf{x})$	Real part 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 $x$
<b>rm</b> (x)	clear the value stored in $x$ ; $\mathbf{rm}(\text{list}=\text{ls}())$ clears all values
Plotting	
$\mathbf{plot}(\mathbf{x}, \mathbf{y}, \mathbf{type}="l", \mathbf{xlab}="X$	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 <i>color</i> (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 <b>paste</b> command
lines(x, y,), points(x, y,)	Plot lines or points on an existing plot; note that you have to start
	the plot with <b>plot</b> (can be a blank line with type="n") and then
	use these; use the <b>legend</b> command to add a legend if desired
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 $labs$ for the bars
hist(x,breaks=20,)	Histogram plot of $\mathbf{x}$ with data broken in the specified number of accually space intervals (e.g. 20)
contour(x, y, z, n) ovols = 10)	Contour plot with playels contours of the matrix $z$ where $x$ and $u$
$\frac{\text{contour}(x,y,z,\text{mevels}=10)}{10}$	z are the locations the grid lines where the z values were computed
	To get filled contours use filled contour Alternative contour
	not commands are available in the lattice package
image(z)	Color map plot based on values of $z$
<b>ndf</b> (file—"fileName ndf")	Create file fileName add to save plot in Use this command before
pur (me= mervanie.pur )	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.
<b>par</b> (mfrow=c(m,n), cex.axis=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
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<b>c</b> (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
$\mathbf{rep}(val, rep)$	A vector of value <i>val</i> repeated <i>rep</i> times
<b>seq</b> (startVal, endVal, by=inc)	A vector from <i>startVal</i> to <i>endVal</i> in increments of <i>inc</i>
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 $v$
sum(v)	Sum of all entries in vector $v$ (also works for matrices)
$\mathbf{cumsum}(\mathbf{v})$	Cumulative sum of vector $v$ at each entry (e.g., if $v =$
	$(a_1, a_2, a_3)$ , cumsum $(v) = (a_1, a_1 + a_2, a_1 + a_2 + a_3)$
$\min(v), \max(v)$	Minimum or maximum value in vector $v$ (also works for ma-
	trices)
mean(v), var(v), sd(v)	Mean, variance, and (sample) standard deviation of vector $v$
cor(v,w)	Correlation of vectors $v$ and $w$
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 $v$
as.data.frame(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
$\mathbf{cbind}(v1, v2,)$	Combine vectors (or matrices) $v1, v2, \dots$ along columns
$\mathbf{rbind}(v1, v2,)$	Combine vectors (or matrices) $v1, v2, \dots$ along rows
nrow(M), ncol(M), 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
t(M)	Transpose of $M$
det(M)	Determinant of $M$
ev = eigen(M)	Eigenvalues ( $ev$ \$values) and eigenvectors ( $ev$ \$vectors) of $M$
M%*%N	Matrix multiplication of $M$ and $N$
M%x%N	Kronecker product of $M$ and $N$ (equivalently, <b>kronecker</b> (M, N))
M%0% $N$	Outer product of $M$ and $N$ (equivalently, <b>outer</b> (M, N))
rowSums(M), colSums(M)	Sum across rows or columns ( <b>sum</b> (M) sums all entries)

Scripts and functions	
# text	Comment ( $text$ is not read by R)
<pre>source("scriptName.R")</pre>	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
<b>print</b> (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 <i>searchMin</i> to <i>searchMax</i>
out = optim(x0, fn)	Find the minimum $(out\$par)$ of function $fn$ given initial guess
	x0
$\mathbf{debug}(\mathrm{fn})$	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; <b>browser</b> and <b>traceback</b> 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
$\mathbf{while}(\mathrm{cond})\{\}$	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, <b>switch</b> 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 <b>lsoda</b>
lsoda(n0, seq(t0,tf,dt), odeFun,	Numerically integrate the function <i>odeFun</i> 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 <b>ode</b> instead of <b>lsoda</b> .
odeFun = function(t, n, parms)	Appropriate structure for a function for use in lsoda: 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 <i>parms</i> using $with(as.list(parms), \{\})$ , and
	need to return $dn$ as a list

Random numbers	
$\mathbf{rnorm}(num, mean=m, sd=s)$	num random normal variables from a distribution with mean $m$
	and standard deviation $s$ . To compute uniform random num-
	bers use <b>runif</b> , Poisson distributed numbers <b>rpoiss</b> , exponen-
	tially distributed numbers <b>rexp</b> , binomially distributed numbers
	rbinom, etc.
dnorm(num, mean=m, sd=s)	Computes the density at $num$ for a normal distribution with
	mean $m$ and standard deviation $s$ . To compute densities for uni-
	form random numbers use <b>dunif</b> , Poisson distributed numbers
	dpoiss, exponentially distributed numbers dexp, binomially dis-
	tributed numbers <b>dbinom</b> , etc.
$\mathbf{pnorm}(num, mean=m, sd=s)$	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 <b>punif</b> , Poisson distributed
	numbers <b>ppoiss</b> , exponentially distributed numbers <b>pexp</b> , bino-
	mially distributed numbers <b>pbinom</b> , 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.
<b>sample</b> (v, num, replace=FALSE)	Sample $num$ entries from the vector $v$ without replacement (or
	replace=TRUE for with replacement)

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

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