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 |
| $\mathbf{rm}(x)$ | clear the value stored in x ; $\mathbf{rm}(\text{list=ls}())$ clears all values |

| 2 () | real the value stored in w, 1111(hot ho()) elected the values |
|---|--|
| 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 |
| 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 |
| hist (x,breaks=20,) | 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. |
| $\mathbf{image}(\mathbf{z})$ | Color map plot based on values of z . |
| pdf (file="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. |
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| 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 start Val to end Val in increments of 1 |
| rep(val, rep) | A vector of value val repeated rep times |
| seq(startVal, endVal, by=inc) | A vector from start Val to end Val 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) |
| cumsum(v) | Cumulative sum of vector v at each entry (e.g., if $v = $ |
| | (a_1, a_2, a_3) , cumsum $(v) = (a_1, a_1 + a_2, a_1 + a_2 + a_3)$ |
| $\min(v), \max(v), \operatorname{range}(v)$ | 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) |
| $\mathbf{which.max}(\mathbf{v})$ | Which entries of v equal the maximum value |
| $\mathbf{rev}(\mathbf{v})$ | Reverse of vector v |
| $\textbf{as.data.frame}(\mathbf{x})$ | 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 <i>Nrows</i> rows and <i>Ncols</i> |
| | 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, $\mathbf{outer}(M, N)$) |
| $\mathbf{rowSums}(\mathbf{M}),\mathbf{colSums}(\mathbf{M})$ | 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 |
| $\mathbf{if}(\text{cond})\{\}\mathbf{else}\{\}$ | 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 |
| | dpoiss, exponentially distributed numbers 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. |
| $\mathbf{summary}(\mathbf{model})$ | 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 |
| predict (model,newdata,type) | 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 <i>data.txt</i> file into a data frame; apply as.matrix |
| | to convert to a matrix |
| 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 |
| \mathbf{FME} | Includes sensitivity analyses for continuous-time models |
| mnormt | Multivariate normals |
| multicore | Parallel processing |
| knitr | Generating reports that integrate R code with text |