Scientific Data Analysis Team

Lecture 4: Writing and Using Functions

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March 11, 2017

Agenda

- Defining functions: Tying related commands into bundles
- Interfaces: Controlling what the function can see and do
- Example: Parameter estimation code

Why Functions?

Data structures tie related values into one object

Functions tie related commands into one object

In both cases: easier to understand, easier to work with, easier to build into larger things

For example

```
# Inputs: vector of numbers (x)
# Outputs: vector with x^2 for small entries, 2|x|-1 for large ones
psi.1 <- function(x) {
  psi <- ifelse(x^2 > 1, 2*abs(x)-1, x^2)
  return(psi)
}
```

Our functions get used just like the built-in ones:

```
z <- c(-0.5,-5,0.9,9)
psi.1(z)
```

```
## [1]  0.25  9.00  0.81 17.00
```

Go back to the declaration and look at the parts:

```
# Inputs: vector of numbers (x)
# Outputs: vector with x^2 for small entries, |x| for large ones
psi.1 <- function(x) {
  psi <- ifelse(x^2 > 1, 2*abs(x)-1, x^2)
  return(psi)
}
```

Interfaces: the **inputs** or **arguments**; the **outputs** or **return value**

Calls other functions `ifelse()`, `abs()`, operators ^ and `>`
could also call other functions we've written

`return()` says what the output is
alternately, return the last evaluation; I like explicit returns better

Comments: Not required by R, but a Very Good Idea
One-line description of purpose; listing of arguments; listing of outputs

What should be a function?

- Things you’re going to re-run, especially if it will be re-run with changes
- Chunks of code you keep highlighting and hitting return on
- Chunks of code which are small parts of bigger analyses
- Chunks which are very similar to other chunks

will say more about design later

Named and default arguments

```r
# Inputs: vector of numbers (x), scale for crossover (c)
# Outputs: vector with x^2 for small entries, 2c|x|-c^2 for large ones
psi.2 <- function(x,c=1) {
  psi <- ifelse(x^2 > c^2, 2*c*abs(x)-c^2, x^2)
  return(psi)
}
```

```r
identical(psi.1(z), psi.2(z,c=1))
```

```
## [1] TRUE
```

Default values get used if names are missing:

```
identical(psi.2(z,c=1), psi.2(z))
```

```
## [1] TRUE
```

Named arguments can go in any order when explicitly tagged:

```
identical(psi.2(x=z,c=2), psi.2(c=2,x=z))
```

```
## [1] TRUE
```

Checking Arguments

Problem: Odd behavior when arguments aren't as we expect

```
psi.2(x=z,c=c(1,1,1,10))
```

```
## [1]  0.25  9.00  0.81 81.00
```

```
psi.2(x=z,c=-1)
```

```
## [1]   0.25 -11.00   0.81 -19.00
```

Solution: Put little sanity checks into the code

```
# Inputs: vector of numbers (x), scale for crossover (c)
# Outputs: vector with x^2 for small entries, 2c|x|-c^2 for large ones
psi.3 <- function(x,c=1) {
  # Scale should be a single positive number
  stopifnot(length(c) == 1,c>0)
  psi <- ifelse(x^2 > c^2, 2*c*abs(x)-c^2, x^2)
  return(psi)
}
```

Arguments to `stopifnot()` are a series of expressions which should all be TRUE; execution halts, with error message, at *first* FALSE (try it!)

What the function can see and do

- Each function has its own environment
- Names here over-ride names in the global environment
- Internal environment starts with the named arguments
- Assignments inside the function only change the internal environment
  There *are* ways around this, but they are difficult and best avoided; see Chambers, ch. 5, if you must
- Names undefined in the function are looked for in the environment the function gets called from
  not the environment of definition

Internal environment examples

```
x <- 7
y <- 9
adder <- function(y) {
  x <- 1
  return(x+y) }
adder(1)
```

```
## [1] 2
```

```
x
```

```
## [1] 7
```

```
y
```

```
## [1] 9
```

Assining value into global environment in function

```r
x <- 7
y <- 9
adder <- function(y) {
  x <<- 1
  return(x+y) }
adder(1)
```

```
## [1] 2
```

```r
x
```

```
## [1] 1
```

```r
y
```

```
## [1] 9
```

Internal environment examples cont'd.

```
circle.area <- function(r) { return(pi*r^2) }
circle.area(c(1,2,3))
```

```
## [1]  3.141593 12.566371 28.274334
```

```
truepi <- pi
pi <- 3   # Valid in 1800s Indiana, or drowned R'lyeh
circle.area(c(1,2,3))
```

```
## [1]  3 12 27
```

```
pi <- truepi      # Restore sanity
circle.area(c(1,2,3))
```

```
## [1]  3.141593 12.566371 28.274334
```

Respect the Interfaces!

Interfaces mark out a controlled inner environment for our code

Interact with the rest of the system only at the interface

Advice: arguments explicitly give the function all the information

Likewise, output should only be through the return value

More Read: More example in the related paper of environment and framework in your course homepage

Example: Fitting a Model

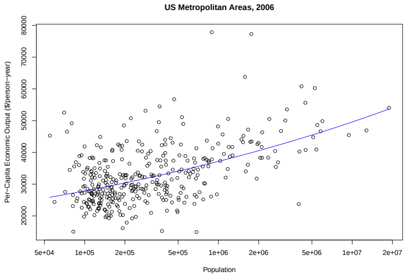
Fact: bigger cities tend to produce more economically per capita
A proposed statistical model (Geoffrey West et al.):

$$Y = y_0 N^a + \text{noise}$$

where Y is the per-capita “gross metropolitan product” of a city, N is its population, and y_0 and a are parameters

Evidence

```r
gmp <- read.table("https://smnajibi.github.io/statcomp/data/gmp.dat")
gmp$pop <- gmp$gmp/gmp$pcgmp
plot(pcgmp~pop, data=gmp, log="x", xlab="Population",
  ylab="Per-Capita Economic Output ($/person-year)",
  main="US Metropolitan Areas, 2006")
curve(6611*x^(1/8),add=TRUE,col="blue")
```



Want to fit the model

$$Y = y_0 N^a + \text{noise}$$

Take $y_0 = 6611$ for today

Approximate the derivative of error w.r.t a and move against it

$$\begin{aligned} MSE(a) &\equiv \frac{1}{n}\sum_{i=1}^{n}(Y_i - y_0 N_i^a)^2 \\ MSE'(a) &\approx \frac{MSE(a+h) - MSE(a)}{h} \\ a_{t+1} - a_t &\propto -MSE'(a) \end{aligned}$$

An actual first attempt at code:

```
maximum.iterations <- 100
deriv.step <- 1/1000
step.scale <- 1e-12
stopping.deriv <- 1/100
iteration <- 0
deriv <- Inf
a <- 0.15
while((iteration < maximum.iterations)&&(deriv > stopping.deriv))
{
  iteration <- iteration + 1
  mse.1 <- mean((gmp$pcgmp - 6611*gmp$pop^a)^2)
  mse.2 <- mean((gmp$pcgmp - 6611*gmp$pop^(a+deriv.step))^2)
  deriv <- (mse.2 - mse.1)/deriv.step
  a <- a - step.scale*deriv
}
list(a=a,iterations=iteration,converged=(iteration < maximum.iterations))
```

What's wrong with this?

- Not *encapsulated*: Re-run by cutting and pasting code — but how much of it? Also, hard to make part of something larger
- *Inflexible*: To change initial guess at a, have to edit, cut, paste, and re-run
- *Error-prone*: To change the data set, have to edit, cut, paste, re-run, and hope that all the edits are consistent
- *Hard to fix*: should stop when *absolute value* of derivative is small, but this stops when large and negative. Imagine having five copies of this and needing to fix same bug on each.

Will turn this into a function and then improve it

First attempt, with logic fix:

```r
estimate.scaling.exponent.1 <- function(a) {
  maximum.iterations <- 100
  deriv.step <- 1/1000
  step.scale <- 1e-12
  stopping.deriv <- 1/100
  iteration <- 0
  deriv <- Inf
  while ((iteration < maximum.iterations) && (abs(deriv) > stopping.deriv)) {
    iteration <- iteration + 1
    mse.1 <- mean((gmp$pcgmp - 6611*gmp$pop^a)^2)
    mse.2 <- mean((gmp$pcgmp - 6611*gmp$pop^(a+deriv.step))^2)
    deriv <- (mse.2 - mse.1)/deriv.step
    a <- a - step.scale*deriv
  }
  fit <- list(a=a,iterations=iteration,
    converged=(iteration < maximum.iterations))
  return(fit)
}
```

Problem: All those magic numbers!

Solution: Make them defaults

```r
estimate.scaling.exponent.2 <- function(a, y0=6611,
  maximum.iterations=100, deriv.step = .001,
  step.scale = 1e-12, stopping.deriv = .01) {
  iteration <- 0
  deriv <- Inf
  while ((iteration < maximum.iterations) && (abs(deriv) > stopping.deriv)) {
    iteration <- iteration + 1
    mse.1 <- mean((gmp$pcgmp - y0*gmp$pop^a)^2)
    mse.2 <- mean((gmp$pcgmp - y0*gmp$pop^(a+deriv.step))^2)
    deriv <- (mse.2 - mse.1)/deriv.step
    a <- a - step.scale*deriv
  }
  fit <- list(a=a,iterations=iteration,
    converged=(iteration < maximum.iterations))
  return(fit)
}
```

Problem: Why type out the same calculation of the MSE twice?
Solution: Declare a function

```
estimate.scaling.exponent.3 <- function(a, y0=6611,
  maximum.iterations=100, deriv.step = .001,
  step.scale = 1e-12, stopping.deriv = .01) {
  iteration <- 0
  deriv <- Inf
  mse <- function(a) { mean((gmp$pcgmp - y0*gmp$pop^a)^2) }
  while ((iteration < maximum.iterations) && (abs(deriv) > stopping.deriv)) {
    iteration <- iteration + 1
    deriv <- (mse(a+deriv.step) - mse(a))/deriv.step
    a <- a - step.scale*deriv
  }
  fit <- list(a=a,iterations=iteration,
    converged=(iteration < maximum.iterations))
  return(fit)
}
```

`mse()` declared inside the function, so it can see `y0`, but it's not added to the global environment

Problem: Locked in to using specific columns of `gmp`; shouldn't have to re-write just to compare two data sets
Solution: More arguments, with defaults

```
estimate.scaling.exponent.4 <- function(a, y0=6611,
  response=gmp$pcgmp, predictor = gmp$pop,
  maximum.iterations=100, deriv.step = .001,
  step.scale = 1e-12, stopping.deriv = .01) {
  iteration <- 0
  deriv <- Inf
  mse <- function(a) { mean((response - y0*predictor^a)^2) }
  while ((iteration < maximum.iterations) && (abs(deriv) > stopping.deriv)) {
    iteration <- iteration + 1
    deriv <- (mse(a+deriv.step) - mse(a))/deriv.step
    a <- a - step.scale*deriv
  }
  fit <- list(a=a,iterations=iteration,
    converged=(iteration < maximum.iterations))
  return(fit)
}
```

Respecting the interfaces: We could turn the **`while()`** loop into a **`for()`** loop, and nothing outside the function would care

```r
estimate.scaling.exponent.5 <- function(a, y0=6611,
  response=gmp$pcgmp, predictor = gmp$pop,
  maximum.iterations=100, deriv.step = .001,
  step.scale = 1e-12, stopping.deriv = .01) {
  mse <- function(a) { mean((response - y0*predictor^a)^2) }
  for (iteration in 1:maximum.iterations) {
    deriv <- (mse(a+deriv.step) - mse(a))/deriv.step
    a <- a - step.scale*deriv
    if (abs(deriv) <= stopping.deriv) { break() }
  }
  fit <- list(a=a,iterations=iteration,
    converged=(iteration < maximum.iterations))
  return(fit)
}
```

What have we done?

The final code is shorter, clearer, more flexible, and more re-usable

Exercise: Run the code with the default values to get an estimate of a; plot the curve along with the data points

Exercise: Randomly remove one data point — how much does the estimate change?

Exercise: Run the code from multiple starting points — how different are the estimates of a?

Summary

- **Functions** bundle related commands together into objects: easier to re-run, easier to re-use, easier to combine, easier to modify, less risk of error, easier to think about
- **Interfaces** control what the function can see (arguments, environment) and change (its internals, its return value)
- **Calling** functions we define works just like calling built-in functions: named arguments, defaults

We will work with many functions after that