Writing and Using Functions

36-350

15 September 2014

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

```
# "Robust" loss function, for outlier-resistant regression
# 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
```

(cont'd.)

Go back to the declaration and look at the parts:

```
# "Robust" loss function, for outlier-resistant regression
# 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

```
# "Robust" loss function, for outlier-resistant regression
# 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)
}
```

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

[1] TRUE

Default Values

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

```
# "Robust" loss function, for outlier-resistant regression
# 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
- ullet 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 <- c("A","C","G","T","U")
adder <- function(y) { x<- x+y; return(x) }
adder(1)</pre>
```

```
## [1] 8

x

## [1] 7

y

## [1] "A" "C" "G" "T" "U"

circle.area <- function(r) { return(pi*r^2) }

circle.area(c(1,2,3))

## [1] 3.142 12.566 28.274

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))</pre>
```

Respect the Interfaces!

[1] 3.142 12.566 28.274

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

Reduces risk of confusion and error Exception: true universals like π

Likewise, output should only be through the return value

More about breaking up tasks and about environments later

Further reading: Herbert Simon, The Sciences of the Artificial

Example: Fitting a Model

Fact: bigger cities tend to produce more economically per capita

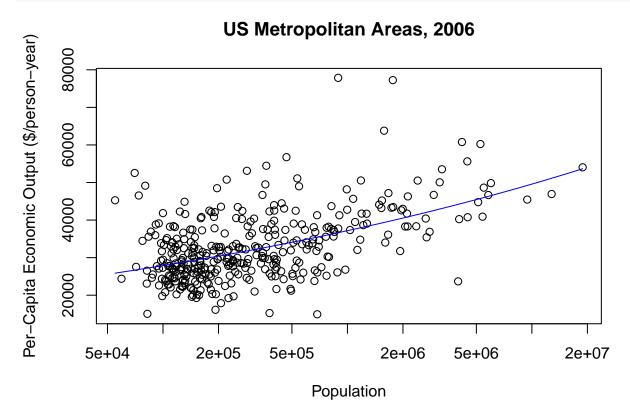
A proposed statistical model (Geoffrey West et al.):

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

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

Evidence

```
gmp <- read.table("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")</pre>
```



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

$$MSE(a) \equiv \frac{1}{n} \sum_{i=1}^{n} (Y_i - y_0 N_i^a)^2$$

$$MSE'(a) \approx \frac{MSE(a+h) - MSE(a)}{h}$$

$$a_{t+1} - a_t \propto -MSE'(a)$$

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))</pre>
## $a
## [1] 0.1258
```

\$iterations ## [1] 58 ## ## \$converged ## [1] TRUE

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

Second Attempt

First attempt, with logic fix:

```
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)</pre>
```

```
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)
}</pre>
```

Third Attempt

Problem: All those magic numbers!

Solution: Make them defaults

```
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)
}</pre>
```

Fourth Attempt

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))</pre>
```

```
return(fit)
}
```

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

Fifth Attempt

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)
}</pre>
```

Sixth Attempt

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

```
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)
}</pre>
```

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

Next time: working with many functions