Writing Functions

James M. Flegal

Agenda

- Defining functions: Tying related commands into bundles
- Interfaces: Controlling what the function can see and do
- Example: Parameter estimation code
- Multiple functions
- Recursion: Making hard problems simpler

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

Example cubic function

```
cube <- function(x) x ^ 3
cube
```

```
## function(x) x ^ 3
```

```
cube(3)
```

```
## [1] 27
```

```
cube(1:10)
```

```
##  [1]    1    8   27   64  125  216  343  512  729 1000
```

```r
cube(matrix(1:8, 2, 4))
```

```
##      [,1] [,2] [,3] [,4]
## [1,]    1   27  125  343
## [2,]    8   64  216  512
```

```r
matrix(cube(1:8), 2, 4)
```

```
##      [,1] [,2] [,3] [,4]
## [1,]    1   27  125  343
## [2,]    8   64  216  512
```

```r
# cube(array(1:24, c(2, 3, 4))) # cube each element in an array
mode(cube)
```

```
## [1] "function"
```

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
```

- 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 `>`, and could also call other functions we've written
- `return()` says what the output is; alternately, return the last evaluation
- Comments are not required by R, but a good idea

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

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 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)
- 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)
```

```
## [1] 8
```

```
x
```

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

```
y
```

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

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

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

```r
truepi <- pi
pi <- 3
circle.area(c(1,2,3))
```

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

```r
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
  - Reduces risk of confusion and error
  - Exception: true universals like π
- Likewise, output should only be through the return value

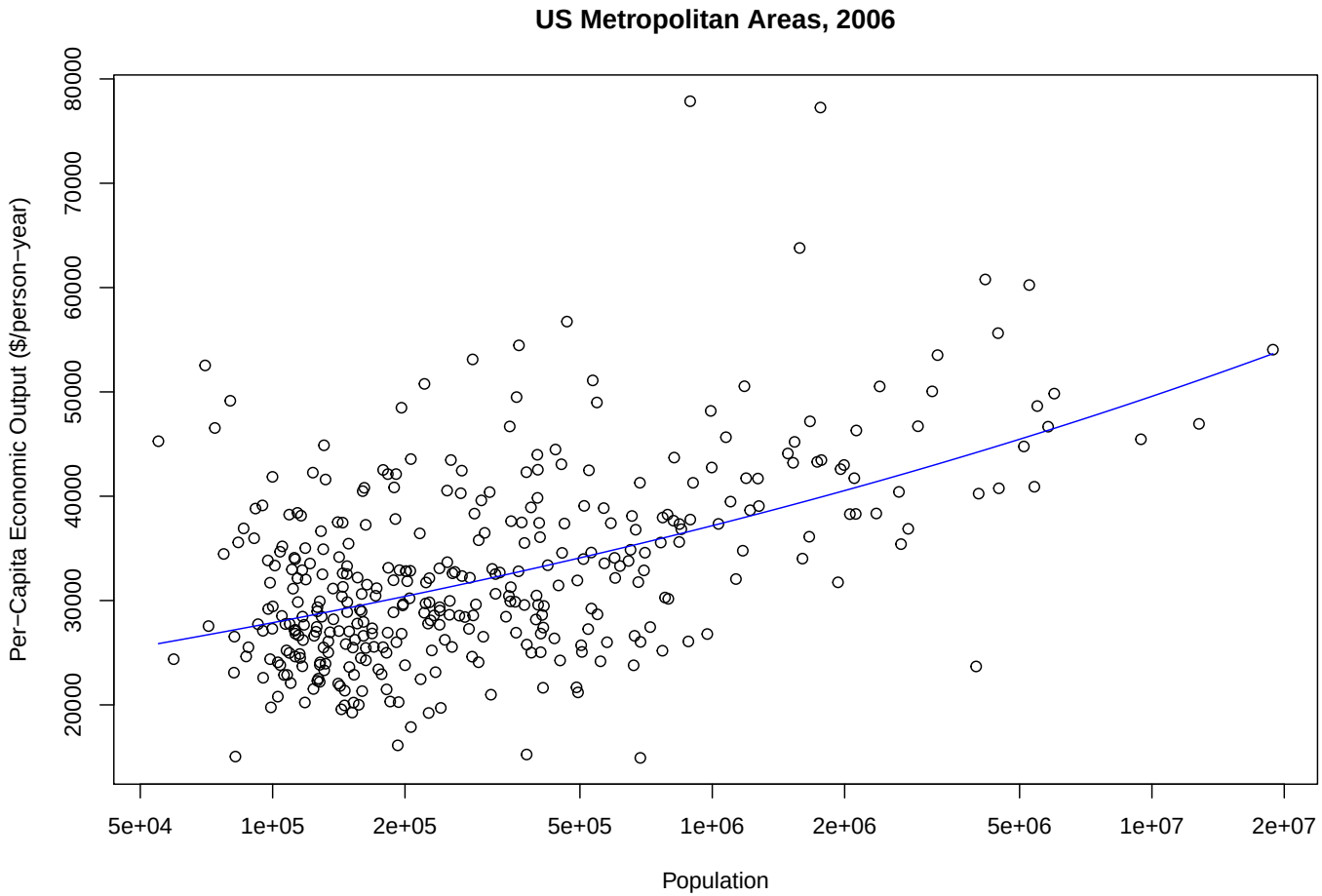
Fitting a Model

- Bigger cities tend to produce more economically per capita
- Proposed statistical model (Geoffrey West et al.) is

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

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

```
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")
```



Fitting a Model

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

- Take $y_0 = 6611$ for now and estimate a by minimizing the mean squared error
- Approximate the derivative of error w.r.t a and move against it

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

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

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

- 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))
```

```
## $a
## [1] 0.1258166
##
## $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

- 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)
    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

```
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 MSE calculation 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

```
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?

- 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?

How We Extend Functions

- Multiple functions: Doing different things to the same object
- Sub-functions: Breaking up big jobs into small ones

Why Multiple Functions?

- Meta-problems
  - You've got more than one problem
  - Your problem is too hard to solve in one step
  - You keep solving the same problems
- Meta-solutions
  - Write multiple functions, which rely on each other
  - Split your problem, and write functions for the pieces
  - Solve the recurring problems once, and re-use the solutions

Writing Multiple Related Functions

- Statisticians want to do lots of things with their models: estimate, predict, visualize, test, compare, simulate, uncertainty, . . .
- Write multiple functions to do these things
- Make the model one object; assume it has certain components

Consistent Interfaces

- Functions for the same kind of object should use the same arguments, and presume the same structure
- Functions for the same kind of task should use the same arguments, and return the same sort of value (to the extent possible)

Keep related things together

- Put all the related functions in a single file
- Source them together
- Use comments to note ***dependencies***

Power-Law Scaling

- Remember the model

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

$$(\text{output per person}) =$$

$$(\text{baseline})(\text{population})^{\text{scaling exponent}} + \text{noise}$$

- Estimated parameters a, y_0 by minimizing the mean squared error
- Exercise: Modify the estimation code from last time so it returns a list, with components `a` and `y0`

Predicting from a Fitted Model

- Predict values from the power-law model

```
# Predict response values from a power-law scaling model
# Inputs: fitted power-law model (object), vector of values at which to make
  # predictions at (newdata)
# Outputs: vector of predicted response values
predict.plm <- function(object, newdata) {
  # Check that object has the right components
  stopifnot("a" %in% names(object), "y0" %in% names(object))
  a <- object$a
  y0 <- object$y0
  # Sanity check the inputs
  stopifnot(is.numeric(a),length(a)==1)
  stopifnot(is.numeric(y0),length(y0)==1)
  stopifnot(is.numeric(newdata))
  return(y0*newdata^a)  # Actual calculation and return
}
```

Predicting from a Fitted Model

```
# Plot fitted curve from power law model over specified range
# Inputs: list containing parameters (plm), start and end of range (from, to)
# Outputs: TRUE, silently, if successful
# Side-effect: Makes the plot
plot.plm.1 <- function(plm,from,to) {
  # Take sanity-checking of parameters as read
  y0 <- plm$y0 # Extract parameters
  a <- plm$a
  f <- function(x) { return(y0*x^a) }
  curve(f(x),from=from,to=to)
  # Return with no visible value on the terminal
  invisible(TRUE)
}
```

Predicting from a Fitted Model

- When one function calls another, use `...` as a meta-argument, to pass along unspecified inputs to the called function:

```
plot.plm.2 <- function(plm,...) {
  y0 <- plm$y0
  a <- plm$a
  f <- function(x) { return(y0*x^a) }
  # from and to are possible arguments to curve()
  curve(f(x), ...)
  invisible(TRUE)
}
```

Sub-Functions

- Solve big problems by dividing them into a few sub-problems
  - Easier to understand, get the big picture at a glance
  - Easier to fix, improve and modify
  - Easier to design
  - Easier to re-use solutions to recurring sub-problems
- Rule of thumb: A function longer than a page is probably too long

Sub-Functions or Separate Functions?

- Defining a function inside another function
  - Pros: Simpler code, access to local variables, doesn't clutter workspace
  - Cons: Gets re-declared each time, can't access in global environment (or in other functions)
  - Alternative: Declare the function in the same file, source them together
- Rule of thumb: If you find yourself writing the same code in multiple places, make it a separate function

Plotting a Power-Law Model

- Our old plotting function calculated the fitted values
- But so does our prediction function

```
plot.plm.3 <- function(plm,from,to,n=101,...) {
  x <- seq(from=from,to=to,length.out=n)
  y <- predict.plm(object=plm,newdata=x)
  plot(x,y,...)
  invisible(TRUE)
}
```

Recursion

- Reduce the problem to an easier one of the same form:

```
my.factorial <- function(n) {
  if (n == 1) {
    return(1)
  } else {
    return(n*my.factorial(n-1))
  }
}
```

Recursion

- Or multiple calls (Fibonacci numbers):

```
fib <- function(n) {
  if ( (n==1) || (n==0) ) {
   return(1)
  } else {
   return (fib(n-1) + fib(n-2))
  }
}
```

- Exercise: Convince yourself that any loop can be replaced by recursion; can you always replace recursion with a loop?

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
- **Multiple functions** let us do multiple related jobs, either on the same object or on similar ones
- **Sub-functions** let us break big problems into smaller ones, and re-use the solutions to the smaller ones
- Recursion is a powerful way of making hard problems simpler