Statistics 360: Advanced R for Data Science

Lecture 10

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References:

- Chapter 25 of Advanced R by Wickham.
- The Rcpp website: http://www.rcpp.org/
- Rcpp gallery: https://gallery.rcpp.org/
- Rcpp quick reference
  https://dirk.eddelbuettel.com/code/rcpp/Rcpp-quickref.pdf

Calling C++ from R with Rcpp

- R is written in C, and so in principle it is possible to write C/C++ code that calls R and R code that calls C/C++.
  - Using R "internals" directly is complicated.
  - A base R function for passing R objects to C/C++ is `.Call`.
  - See the chapter "System and foreign language interfaces" in the "Writing R Extensions" manual.
- Rcpp provides a more user-friendly interface with C++.
  - Allows you to write C++ functions that can be called from R
  - Use it to speed up code that runs too slowly in R.
  - Of the 17345 packages on CRAN, 2385 (or more) use Rcpp
- This is a brief intro; much more info at http://www.rcpp.org/ and elsewhere on the internet.
- Warning: This lecture will be too simplified for those with C++ experience, and information overload for those without.

Use cases

- Unavoidable loops (can't avoid by vectorizing).
- Many (e.g., millions) of function calls, such as in a recursive algorithm.
  - Less overhead in C++ compared to R.
- Require advanced data structures and algorithms that are available in a C++ library, such as the Standard Template Library(STL), but not in R.
- And many more . . .

Prerequisites

- Install and load the Rcpp package

```r
# install.packages("Rcpp")
library(Rcpp)
```

- Install a working C++ compiler. To get it:
  - On Windows, install Rtools.
  - On Mac, install Xcode.
  - On Linux, `sudo apt-get install r-base-dev`

Getting started (section 25.2)

- First example:

```r
cppFunction('int add(int x, int y, int z) {
  int sum = x + y + z;
  return sum;
}')
# add works like a regular R function
add
```

```
## function (x, y, z)
## .Call(<pointer: 0x102ca00c0>, x, y, z)
```

```r
add(1, 2, 3)
```

```
## [1] 6
```

- Rcpp (i) compiles the C++ code (note lag) and (ii) constructs the R function `add()` that will call this compiled code.
- The above defines a function "inline"; it is also possible to "source" C++ code (more later).

The plan

- Start simple and work up, writing functions with:
  - no inputs and a scalar output
  - scalar input and scalar output
  - vector input and scalar output
  - vector input and vector output
  - matrix input and vector output
- Keep an eye out for differences, such as the need to declare the type of objects.

No inputs, scalar output

- R:

```
one <- function() 1L # recall that 1L is integer 1
```

- Rcpp (notice single quotes):

```
cppFunction('int one() {
  return 1;
}')
one()
```

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

C++ differences

- Don't use assignment to create functions.
- Declare the type of output the function returns; e.g., a scalar integer (`int`).
- C++ has true scalars, with types `double`, `int`, `String`, and `bool`.
- A return statement is **required**
- Every statement is terminated by a `;`.

Scalar input and output

- A scalar version of the sign() function which returns 1, 0 or -1 for positive, zero or negative input:

```
signR <- function(x) {
  if (x > 0) { 1 } else if (x == 0) { 0 } else { -1 }
}

cppFunction('int signC(int x) {
  if (x > 0) {
    return 1;
  } else if (x == 0) {
    return 0;
  } else {
    return -1;
  }
}')
signC(-100)
```

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

Notes

- In addition to declaring the type of the output, we must declare the type of the input.
- Logicals and `if-else` are the same.

Vector input and scalar output

```r
sumR <- function(x) {
  total <- 0
  for (i in seq_along(x)) {
    total <- total + x[i]
  }
  total
}
cppFunction('double sumC(NumericVector x) {
  int n = x.size();
  double total = 0;
  for(int i = 0; i < n; i++) {
    total += x[i];
  }
  return total;
}')
```

```r
set.seed(1)
x <- rnorm(1e5)
bench::mark(sumR(x),sumC(x),sum(x)) # recall benchmarking pkg be
```

```
## # A tibble: 3 x 6
##   expression      min   median `itr/sec` mem_alloc `gc/sec`
##   <bch:expr> <bch:tm> <bch:tm>     <dbl> <bch:byt>    <dbl>
## 1 sumR(x)      1.43ms   1.47ms      678.    3.99MB        0
## 2 sumC(x)     92.78us  94.55us    10464.    2.49KB        0
## 3 sum(x)     153.59us 156.13us     6372.        0B        0
```

Notes

- The input (R vector) in this example is of type `NumericVector`, which is a C++ class defined by Rcpp.
  - Other R vector types are `IntegerVector`, `CharacterVector`, and `LogicalVector`.
- The `.size()` method of a vector returns the length as an integer.
- Notice the syntax of `for()`: `for(initial condn; check condn; increment)`.
  - In this case we initialise by creating variable i with value 0.
  - Before each iteration we check that `i < n`, and terminate if not.
  - After each iteration, increment i by one, using ++.
- C++ uses zero-based indexing, 0,. . . n-1 (!!!)
- += increments "in-place"

Vector input, vector output

- Note: In the following, `NumericVector out(n)` is a constructor.

```
pdistR <- function(x, ys) { sqrt((x - ys) ^ 2) }
cppFunction('NumericVector pdistC(double x, NumericVector ys) {
  int n = ys.size();
  NumericVector out(n);

  for(int i = 0; i < n; ++i) {
    out[i] = sqrt(pow(ys[i] - x, 2.0)); //  pow() vs ^{}
  }
  return out;
}')
pdistC(10,6:15)
```

```
##  [1] 4 3 2 1 0 1 2 3 4 5
```

```
try(pdistC(1:3, 6:15) )
```

```
## Error in pdistC(1:3, 6:15) : Expecting a single value: [extent=3].
```

Copying with clone

- In R we use assignment to copy vectors.
- In C++ with Rcpp copy an existing vector with the `clone()` function; e.g., `NumericVector zs = clone(ys)`.

Using sourceCpp

- For functions of more than a few lines it is more convenient to define them in a source file and use `sourceCpp()` to link them to R.
- Source files must end in `.cpp` and start with the header

```
#include <Rcpp.h>
using namespace Rcpp;
```

- The `File -> New File -> C++ file` feature of RStudio generates a skeleton to get you started; see `lec10_1.cpp`.

```r
sourceCpp("lec10_1.cpp") # See source file
```

```
##
## > timesTwo(42)
## [1] 84
```

```r
timesTwo(3:6)
```

```
## [1]  6  8 10 12
```

Other classes (Section 25.3)

- Rcpp provides wrappers to other base data type.
- The text focusses on lists/data frames, functions and attributes.

List input, including S3 classes

- Generally more useful for output than input, because C++ needs to know classes of list components in advance.
- For use as input, you can convert components to C++ equivalents with `as()`.
  - See the source file `lec10_2.cpp` for the following example.

```
sourceCpp("lec10_2.cpp")
mod <- lm(mpg ~ wt, data = mtcars)
mpe(mod) # function defined in lec10_2.cpp
```

```
## [1] -0.01541615
```

Aside: Primer on C++ templates

- Few details here, just a few words so we recognize function and class templates when we see them.
- C++ template functions allow programmers to write code that takes a generic argument.
  - A template function `func<T>()` takes template parameter `T` that can be the type of the function inputs and/or output. For a given `T`, the compiler generates a function specific to that type.
  - Examples: `as<NumericVector>(SEXP R)` is a function that takes an R expression (SEXP) as input and returns a `NumericVector`; `as<CharacterVector>(SEXP R)` returns a `CharacterVector`; etc.
- Data structures can also be templated; e.g., the C++ Standard Template Library (STL) defines a `vector` class that is like a generic container, with methods for inserting, re-sizing, etc.
  - You can create a vector of `int`s with `vector<int>`, etc.
- Defining your own template functions and classes is beyond the scope of this class.

Functions

- So far we have been using Rcpp to call C++ functions from R, but we can also call R functions from C++.
- Use type `Function` to input R functions and type `RObject` to hold general input/output.

```
sourceCpp("lec10_3.cpp") # see source file
set.seed(123)
x <- rnorm(100)
callFunction(x,fivenum)
```

```
## [1] -2.30916888 -0.49667731  0.06175631  0.69499808  2.18733299
```

```
callWithOne(function(x) x+1)
```

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

```
fit <- lm_in_C(formula(mpg~disp),mtcars,lm)
summary(fit)$coef
```

```
##                Estimate  Std. Error   t value     Pr(>|t|)
## (Intercept) 29.59985476 1.229719515 24.070411 3.576586e-21
## disp        -0.04121512 0.004711833 -8.747152 9.380327e-10
```

A warning from the Rcpp developers

- Occasional R function calls from C++ are OK, but don't call repeatedly.
- From https://gallery.rcpp.org/articles/r-function-from-c++/ :
  Calling a function is simple and tempting. It is also slow as there are overheads involved. And calling it repeatedly from inside your C++ code, possibly buried within several loops, is outright silly. This has to be slower than equivalent C++ code, and even slower than just the R code (because of the marshalling of data). Do it when it makes sense, and not simply because it is available.
- Consider instead accessing R functionality from the GNU Scientific Library https://www.gnu.org/software/gsl/doc/html/index.html *via* the RcppGSL package, or one of the 50 or so other Rcpp* C/C++ library interfaces.

Attributes

- In R we get and set attributes with `attr()`; e.g.,

```
out <- c(1,2,3)
names(out) <- c("a","b","c")
attr(out,"my-attr") <- "my-value"
attr(out,"class") <- "my-class" # or class(out) <- "my-class"
out
```

```
## a b c
## 1 2 3
## attr(,"my-attr")
## [1] "my-value"
## attr(,"class")
## [1] "my-class"
```

Attributes with Rcpp

- From Rcpp, get and set R object attributes with the `.names()` and .attr()‘ methods for R vector types.

```
sourceCpp("lec10_4.cpp") # see source file
attribs()
```

```
## a b c
## 1 2 3
## attr(,"my-attr")
## [1] "my-value"
## attr(,"class")
## [1] "my-class"
```

C++ Standard Template Library (Section 25.5)

- References: Text, section 25.5, and https://www.cppreference.com/Cpp_STL_ReferenceManual.pdf
- Rcpp gives us access to the data structures and algorithms provided by C++ libraries like the Standard Template Library (STL).
- We'll cover some STL basics.
  - Data structures
  - Iterators
  - Algorithms
- The theme of the STL is abstraction: Implementations of algorithms encapsulate the logic and operate on generic data structures that we think of as "containers", capable of holding any kind of data.
- Note: Many of the data structures and algorithms that originated in the STL have made their way into the C++ Standard Library; this is true of all of those used in this lecture.

Lists in R are generic containers

- In R, lists can be thought of as generic containers that generalize atomic vectors to hold arbitrary data structures.

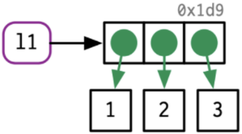


Figure 1: Lists as generic containers

- In R, list elements can be accessed by index, in the same way as vectors (in fact, we refer to lists as vectors); this is called “random access”.

Container performance tradoffs

- The STL offers different containers with different performance characteristics. For example:
  - vectors allow fast random access, but are slow for insertion/deletion
  - lists (not R lists) allow fast insertion/deletion, but access to elements requires traversal of the container, starting at one end.
- Unlike R lists, STL vector and list elements must be of the same type.
  - E.G., create a vector of integers of length 9 with `vector<int> myvec (9)`
  - Rcpp data structures like `NumericVector` are essentially typed STL vectors (`NumericVector` is `vector<double>`).
- Algorithms can be written to work on multiple container types by abstracting how we access elements. The abstraction is called an iterator.

Using iterators

- We will use the following three features of iterators:
  1. Advance with `++` or `--`.
  2. Get the value they refer to, or dereference, with `*`.
  3. Compare with `==` and `!=`.
- The following code snippets compare a sum function that uses indexing to one that uses an iterator to loop over the vector.

```
#include <Rcpp.h>
using namespace Rcpp;
// [[Rcpp::export]]
double sumC(NumericVector x) {
  int n = x.size();
  double total = 0;
  for(int i = 0; i < n; ++i) {
    total += x[i];
  }
  return total;
}
// [[Rcpp::export]]
double sum3(NumericVector x) {
  double total = 0;
  NumericVector::iterator it;
  for(it = x.begin(); it != x.end(); ++it) {
    total += *it;
  }
  return total;
}
```

- At any given time, the iterator will “refer” (point) to an element of the container.
- We initialize to refer to the first element of the container `x` with `x.begin()` and will stop iterating when the iterator refers to the last element `x.end()`.
- `++it` advances the iterator to refer to the next element of the container.
- `*it` gets the container element that `it` currently refers to.

Algorithms

- Algorithms in the STL often input or output iterators.
- The script `lec10_5.cpp` gives an example from the text.
  - Implements R's `findInterval()` function that takes a numeric vector `x` and vector of breakpoints `breaks` as input and returns the bin defined by `breaks` that each element of `x` is in.

```
sourceCpp("lec10_5.cpp")
findInterval2(x=c(-1.5,-.5,.5,1.5),breaks=c(-1,0,1))
```

```
## [1] 0 1 2 3
```

- Iterates over input `x` with iterator `it` and over output vector `out` with iterator `out_it`.
  - Call `upper_bound()` algorithm from the STL (also in C++ Std Lib) to search `breaks` for the first element greater than `*it`. `upper_bound()` returns an iterator `pos` over the vector `breaks`.
  - Calculate bin (interval) number as distance from start of `breaks` to `pos`.

Case Studies (Section 25.6)

- See the Gibbs sampler and vectorization examples in Section 25.6 of the text
- We'll do a different case study.

Case Study: Metropolis algorithm

- The Metropolis-Hastings (MH) algorithm is an important tool for drawing (dependent) samples from a distribution known only up to a constant.
  - A Markov chain Monte Carlo (MCMC) algorithm that reinvigorated Bayesian statistics in the early 2000s.
  - We will implement a simplified version of the MH algorithm known as the Metroplois algorithm.
- Reference for this demo is Matthew Stephens' "Five Minute Stats" site:
  - Introduction to the Metropolis-Hastings algorithm
    https://stephens999.github.io/fiveMinuteStats/MH_intro.html
  - Example implementations in R
    https://stephens999.github.io/fiveMinuteStats/MH-examples1.html

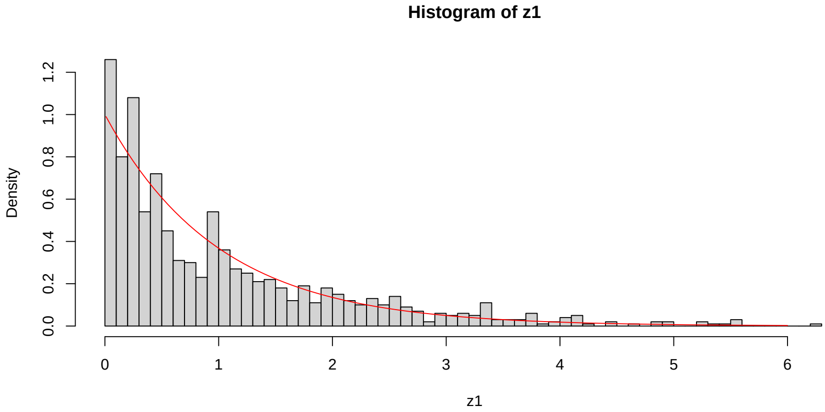
Example Metropolis algorithm

- Problem: sample from an exponential distribution with mean 1.
  - Simple illustration – we know how to do this without MCMC.
- R code to implement the algorithm is as follows

```
target = function(x){
  if(x<0){ return(0) } else { return( exp(-x))}
}
easyMCMC_R = function(niter, startval, proposalsd){
  x = rep(0,niter)
  x[1] = startval
  for(i in 2:niter){
    currentx = x[i-1]
    proposedx = rnorm(1,mean=currentx,sd=proposalsd)
    A = target(proposedx)/target(currentx)
    if(runif(1)<A){
      x[i] = proposedx #accept move with probability min(1,A)
    } else {
      x[i] = currentx #otherwise "reject" move, and stay where we are
    }
  }
  return(x)
}
```

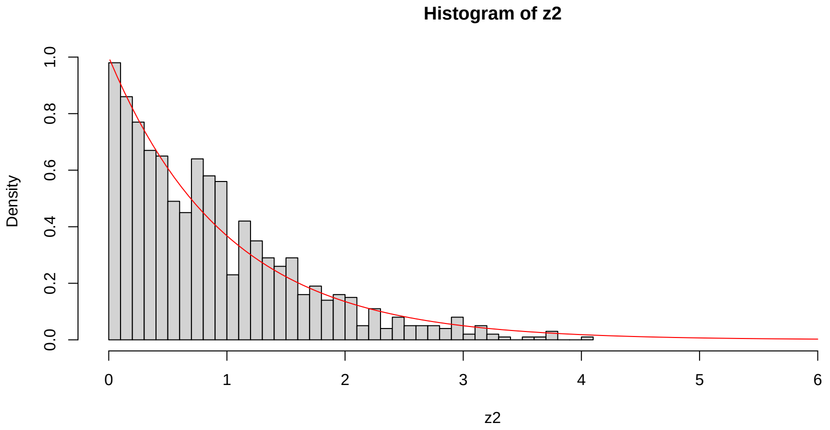
Test out easyMCMC

```
set.seed(123)
N <- 1000; startval <- 3; proposalsd <- 1
z1=easyMCMC_R(N,startval,proposalsd)
hist(z1,nclass=50,freq=FALSE,xlim=c(0,6.5))
xx <- seq(from=0.01,to=6,length=100)
lines(xx,exp(-xx),col="red")
```



Rcpp version

```
sourceCpp("lec10_MCMC1.cpp")
z2 <- easyMCMC_C(N,startval,proposalsd)
hist(z2,nclass=50,freq=FALSE,xlim=c(0,6.5))
lines(xx,exp(-xx),col="red")
```



Benchmark the two implementations

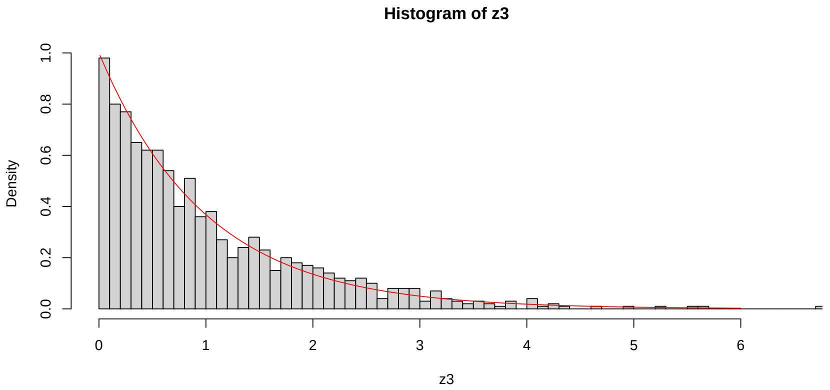
- The C++ version runs about 20 times faster.
- For more complex problems, MCMC algorithms need to run for millions of iterations, so 20-times speedup is good (think one day *vs* three weeks run-time).

```
bench::mark(easyMCMC_R(N,startval,proposalsd),
            easyMCMC_C(N,startval,proposalsd),
            check=FALSE) # don't check equality of function calls
```

```
## # A tibble: 2 x 6
##   expression                                min   median `itr/sec` mem_alloc
##   <bch:expr>                           <bch:tm> <bch:tm>     <dbl> <bch:byt>
## 1 easyMCMC_R(N, startval, proposalsd)    2.06ms   2.43ms      410.    4.87MB
## 2 easyMCMC_C(N, startval, proposalsd) 123.29us 133.46us     7361.   14.48KB
## # ... with 1 more variable: gc/sec <dbl>
```

Compare to R's `rexp()` random exponential generator

```
z3 <- rexp(1000)
hist(z3,nclass=50,freq=FALSE,xlim=c(0,6.5))
lines(xx,exp(-xx),col="red")
```



Rcpp in R packages (Section 25.7)

- Your .cpp files can also be included in a package.
- Call `devtools::use_rcpp()` from your package's RStudio project to get started
  - Compiled code goes in a `src` directory.
  - Rcpp is added to the "Imports" and "LinkingTo" fields of the DESCRIPTION file.
  - And more ...

```
> devtools::use_rcpp()
 Creating 'src/'
 Adding '*.o', '*.so', '*.dll' to 'src/.gitignore'
 Copy and paste the following lines into 'R/mars-package.R':
  ## usethis namespace: start
  #' @useDynLib mars, .registration = TRUE
  ## usethis namespace: end
  NULL
  [Copied to clipboard]
 Adding 'Rcpp' to LinkingTo field in DESCRIPTION
 Adding 'Rcpp' to Imports field in DESCRIPTION
 Copy and paste the following lines into 'R/mars-package.R':
  ## usethis namespace: start
  #' @importFrom Rcpp sourceCpp
  ## usethis namespace: end
  NULL
  [Copied to clipboard]
 Writing 'src/code.cpp'
 Modify 'src/code.cpp'
```

Topics not covered

- Missing values (Section 25.4)