Higher-Performance R via C++

Part 1: Introduction

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Overview

What Are We Doing Today and Tomorrow?

High-level motivation: Three main questions

- Why ? *Several reasons discussed next*
- How ? *Rcpp details, usage, tips, …*
- What ? *We will cover examples.*

Focus on R and C++

- R: Our starting point
- C++: Our extension approach
- *why*, *how*, *tricks*, ...

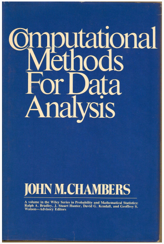
Before the Why/How/What

Maybe some mutual introductions?

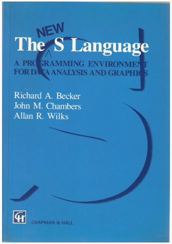
- Your background (academic, industry, …)
- R experience (beginner, intermediate, advanced, …)
- Created / modified any R packages ?
- C and/or C++ experience ?
- Main interest in Rcpp: speed, extensions, …, ?
- Following `rcpp-devel` or `r-devel` ?

Overview: Why R?

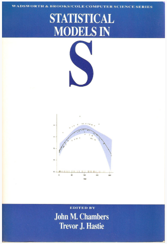
Why R? : *Programming with Data*



Chambers, *Computational Methods for Data Analysis*. Wiley, 1977.



Becker, Chambers, and Wilks. *The New S Language*. Chapman & Hall, 1988.



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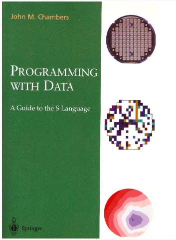
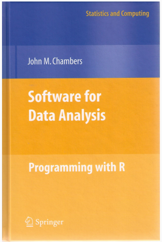


Chambers. *Programming with Data*. Springer, 1998.



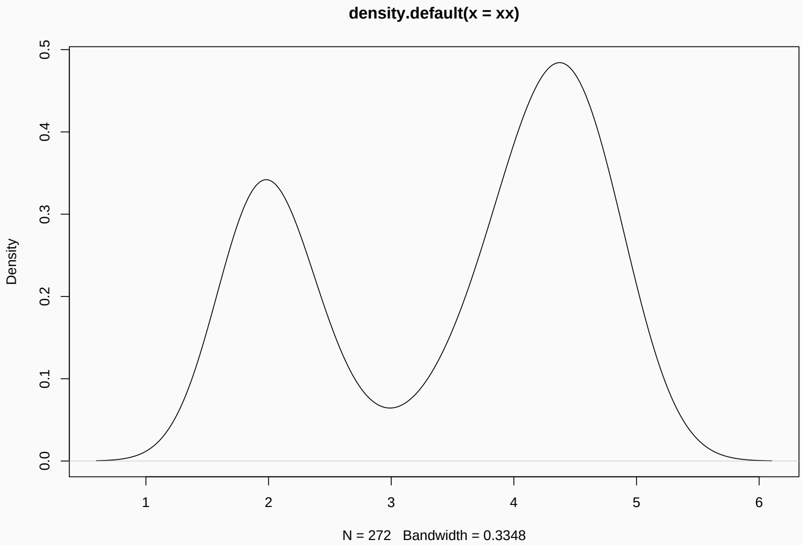
Chambers. *Software for Data Analysis: Programming with R*. Springer, 2008

Thanks to John Chambers for sending me high-resolution scans of the covers of his books.

A Simple Example

```
xx <- faithful[,"eruptions"]
fit <- density(xx)
plot(fit)
```

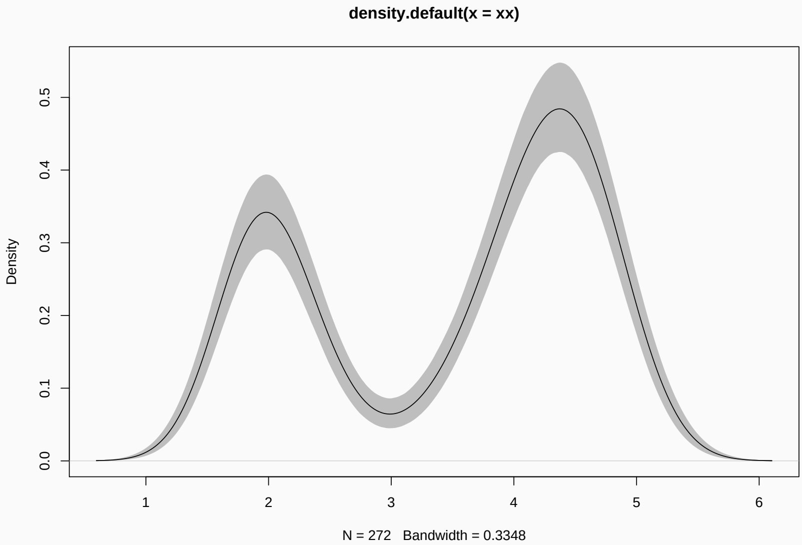
A Simple Example



A Simple Example - Refined

```r
xx <- faithful[,"eruptions"]
fit1 <- density(xx)
fit2 <- replicate(10000, {
    x <- sample(xx,replace=TRUE);
    density(x, from=min(fit1$x), to=max(fit1$x))$y
})
fit3 <- apply(fit2, 1, quantile,c(0.025,0.975))
plot(fit1, ylim=range(fit3))
polygon(c(fit1$x,rev(fit1$x)), c(fit3[1,],rev(fit3[2,])),
    col='grey', border=F)
lines(fit1)
```

A Simple Example - Refined



So Why R?

R enables us to

- work interactively
- explore and visualize data
- access, retrieve and/or generate data
- summarize and report into pdf, html, …

making it the key language for statistical computing, and a preferred environment for many data analysts.

So Why R?

R has always been extensible via

- **C** via a bare-bones interface described in *Writing R Extensions*
- **Fortran** which is also used internally by R
- **Java via** `rJava` by Simon Urbanek
- **C++** but essentially at the bare-bones level of C

So while *in theory* this always worked – it was tedious *in practice*

Why Extend R?

Chambers (2008), opens Chapter 11 *Interfaces I: Using C and Fortran*:

> *Since the core of R is in fact a program written in the C language, it's not surprising that the most direct interface to non-R software is for code written in C, or directly callable from C. All the same, including additional C code is a serious step, with some added dangers and often a substantial amount of programming and debugging required. You should have a good reason.*

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Why Extend R?

Chambers proceeds with this rough map of the road ahead:

- Against:
  - It's more work
  - Bugs will bite
  - Potential platform dependency
  - Less readable software
- In Favor:
  - New and trusted computations
  - Speed
  - Object references

Why Extend R?

The *Why?* boils down to:

- **speed** Often a good enough reason for us … and a focus for us in this workshop.
- **new things** We can bind to libraries and tools that would otherwise be unavailable in R
- **references** Chambers quote from 2008 foreshadowed the work on the new *Reference Classes* now in R and built upon via Rcpp Modules, Rcpp Classes (and also RcppR6)

Overview: Why C++?

Why C++?

- Asking Google leads to about 52 million hits.
- Wikipedia: *C++ is a statically typed, free-form, multi-paradigm, compiled, general-purpose, powerful programming language*
- C++ is industrial-strength, vendor-independent, widely-used, and *still evolving*
- In science & research, one of the most frequently-used languages: If there is something you want to use / connect to, it probably has a C/C++ API
- As a widely used language it also has good tool support (debuggers, profilers, code analysis)

Why C++?

Scott Meyers: *View C++ as a federation of languages*

- *C* provides a rich inheritance and interoperability as Unix, Windows, … are all build on C.
- *Object-Oriented C++* (maybe just to provide endless discussions about exactly what OO is or should be)
- *Templated C++* which is mighty powerful; template meta programming unequalled in other languages.
- *The Standard Template Library* (STL) is a specific template library which is powerful but has its own conventions.
- *C++11* (and C++14 and beyond) add enough to be called a fifth language.

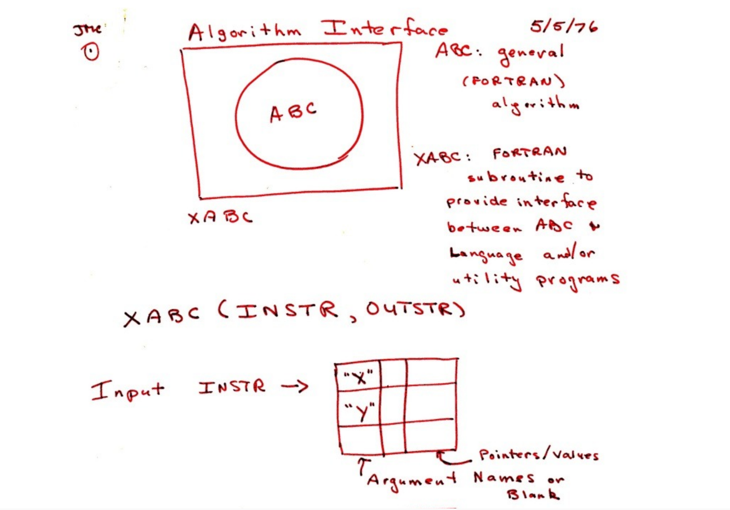
NB: Meyers original list of four languages appeared years before C++11.

Why C++?

- Mature yet current
- Strong performance focus:
  - *You don't pay for what you don't use*
  - *Leave no room for another language between the machine level and C++*
- Yet also powerfully abstract and high-level
- C++11 is a big deal giving us new language features
- While there are complexities, Rcpp users are mostly shielded

Overview: Vision

Bell Labs, May 1976



JMC ①

Algorithm Interface 5/5/76

ABC

XABC

ABC: general (FORTRAN) algorithm

XABC: FORTRAN subroutine to provide interface between ABC & language and/or utility programs

XABC (INSTR, OUTSTR)

Input INSTR →

"X"

"Y"

Pointers/Values

Argument Names or Blank

Interface Vision

R offers us the best of both worlds:

- **Compiled** code with
    - Access to proven libraries and algorithms in C/C++/Fortran
    - Extremely high performance (in both serial and parallel modes)
- **Interpreted** code with
    - An accessible high-level language made for *Programming with Data*
    - An interactive workflow for data analysis
    - Support for rapid prototyping, research, and experimentation

Why Rcpp?

- *Easy to learn* as it really does not have to be that complicated – we will see numerous few examples
- *Easy to use* as it avoids build and OS system complexities thanks to the R infrastrucure
- *Expressive* as it allows for *vectorised* C++ using *Rcpp Sugar*
- *Seamless* access to all R objects: vector, matrix, list, S3/S4/RefClass, Environment, Function, …
- *Speed gains* for a variety of tasks Rcpp excels precisely where R struggles: loops, function calls, …
- *Extensions* greatly facilitates access to external libraries using eg *Rcpp modules*

Overview: Speed

Speed Example 1 (due to Christian Robert)

Five different ways to compute $1/(1+x)$:

```
f <- function(n, x=1) for(i in 1:n) x <- 1/(1+x)
g <- function(n, x=1) for(i in 1:n) x <- (1/(1+x))
h <- function(n, x=1) for(i in 1:n) x <- (1+x)^(-1)
j <- function(n, x=1) for(i in 1:n) x <- {1/{1+x}}
k <- function(n, x=1) for(i in 1:n) x <- 1/{1+x}
library(rbenchmark)
N <- 1e5
benchmark(f(N,1),g(N,1),h(N,1),j(N,1),k(N,1),order="relati
```

Speed Example 1 (due to Christian Robert)

```
##       test replications elapsed relative
## 5 k(N, 1)          100   6.435    1.000
## 1 f(N, 1)          100   6.609    1.027
## 2 g(N, 1)          100   7.757    1.205
## 4 j(N, 1)          100   7.882    1.225
## 3 h(N, 1)          100  11.766    1.828
```

Speed Example 1 (due to Christian Robert)

Adding a C++ variant is easy:

```
cppFunction("
    double m(int n, double x) {
        for (int i=0; i<n; i++)
             x = 1 / (1+x);
        return x;
    }"
)
```

(We will learn more about `cppFunction()` later).

Speed Example 1 (due to Christian Robert)

```
##       test replications elapsed relative
## 6 m(N, 1)          100   0.170    1.000
## 1 f(N, 1)          100   6.854   40.318
## 5 k(N, 1)          100   7.811   45.947
## 4 j(N, 1)          100   9.183   54.018
## 2 g(N, 1)          100   9.489   55.818
## 3 h(N, 1)          100  11.725   68.971
```

Speed Example 2 (due to StackOverflow)

Consider a function defined as

$$\mathsf{f}(n) \quad \text{such that} \quad \begin{cases} n & \text{when} \quad n < 2 \\ \mathsf{f}(n-1) + \mathsf{f}(n-2) & \text{when} \quad n \geq 2 \end{cases}$$

Speed Example 2 (due to StackOverflow)

R implementation and use:

```
f <- function(n) {
    if (n < 2) return(n)
    return(f(n-1) + f(n-2))
}

## Using it on first 11 arguments
sapply(0:10, f)
```

```
##  [1]  0  1  1  2  3  5  8 13 21 34 55
```

Speed Example 2 (due to StackOverflow)

Timing:

```
library(rbenchmark)
benchmark(f(10), f(15), f(20))[,1:4]
```

```
##     test replications elapsed relative
## 1 f(10)          100   0.030    1.000
## 2 f(15)          100   0.335   11.167
## 3 f(20)          100   3.517  117.233
```

Speed Example 2 (due to StackOverflow)

```
int g(int n) {
    if (n < 2) return(n);
    return(g(n-1) + g(n-2));
}
```

deployed as

```
Rcpp::cppFunction("int g(int n) {
   if (n < 2) return(n);
   return(g(n-1) + g(n-2)); }")
sapply(0:10, g)
```

```
##  [1]  0  1  1  2  3  5  8 13 21 34 55
```

Speed Example 2 (due to StackOverflow)

Timing:

```
Rcpp::cppFunction("int g(int n) {
   if (n < 2) return(n);
   return(g(n-1) + g(n-2)); }")
library(rbenchmark)
benchmark(f(20), g(20), order="relative")[,1:4]
```

```
##    test replications elapsed relative
## 2 g(20)          100   0.011    1.000
## 1 f(20)          100   3.776  343.273
```

A nice gain of a few orders of magnitude.

Another Angle on Speed

Run-time performance is just one example.

Time to code is another metric.

We feel quite strongly that helps you code more succinctly, leading to fewer bugs and faster development.

A good environment helps. RStudio integrates R and C++ development quite nicely (eg the compiler error message parsing is very helpful) and also helps with package building.

What Next ?

Hands-on

Programming with C++

- C++ Basics
- Debugging
- Best Practices

and then on to Rcpp itself

C++ Basics

Compiled not Interpreted

Need to compile and link

```
#include <cstdio>

int main(void) {
    printf("Hello, world!\n");
    return 0;
}
```

Compiled not Interpreted

Or streams output rather than `printf`

```
#include <iostream>

int main(void) {
    std::cout << "Hello, world!" << std::endl;
    return 0;
}
```

Compiled not Interpreted

`g++ -o` will compile and link

We will now look at an examples with explicit linking.

Compiled not Interpreted

```
#include <cstdio>

#define MATHLIB_STANDALONE
#include <Rmath.h>

int main(void) {
    printf("N(0,1) 95th percentile %9.8f\n",
           qnorm(0.95, 0.0, 1.0, 1, 0));
}
```

Compiled not Interpreted

We may need to supply:

- *header location* via `-I`,
- *library location* via `-L`,
- *library* via `-llibraryname`

```
g++ -I/usr/include -c qnorm_rmath.cpp
g++ -o qnorm_rmath qnorm_rmath.o -L/usr/lib -lRmath
```

Statically Typed

- R is dynamically typed: `x <- 3.14; x <- "foo"` is valid.
- In C++, each variable must be declared before first use.
- Common types are `int` and `long` (possibly with `unsigned`), `float` and `double`, `bool`, as well as `char`.
- No standard string type, though `std::string` is close.
- All these variables types are scalars which is fundamentally different from R where everything is a vector.
- `class` (and `struct`) allow creation of composite types; classes add behaviour to data to form `objects`.
- Variables need to be declared, cannot change

C++ Basics: A Better C

C++ is a Better C

- control structures similar to what R offers: `for`, `while`, `if`, `switch`
- functions are similar too but note the difference in positional-only matching, also same function name but different arguments allowed in C++
- pointers and memory management: very different, but lots of issues people had with C can be avoided via STL (which is something Rcpp promotes too)
- sometimes still useful to know what a pointer is …

Object-Oriented

This is a second key feature of C++, and it does it differently from S3 and S4.

```
struct Date {
    unsigned int year;
    unsigned int month;
    unsigned int day
};

struct Person {
    char firstname[20];
    char lastname[20];
    struct Date birthday;
    unsigned long id;
};
```

Object-Oriented

Object-orientation in the C++ sense matches data with code operating on it:

```
class Date {
private:
    unsigned int year
    unsigned int month;
    unsigned int date;
public:
    void setDate(int y, int m, int d);
    int getDay();
    int getMonth();
    int getYear();
}
```

Generic Programming and the STL

The STL promotes *generic* programming.

For example, the sequence container types `vector`, `deque`, and `list` all support

- `push_back()` to insert at the end;
- `pop_back()` to remove from the front;
- `begin()` returning an iterator to the first element;
- `end()` returning an iterator to just after the last element;
- `size()` for the number of elements;

but only `list` has `push_front()` and `pop_front()`.

Other useful containers: `set`, `multiset`, `map` and `multimap`.

Generic Programming and the STL

Traversal of containers can be achieved via *iterators* which require suitable member functions `begin()` and `end()`:

```
std::vector<double>::const_iterator si;
for (si=s.begin(); si != s.end(); si++)
    std::cout << *si << std::endl;
```

Generic Programming and the STL

Another key STL part are *algorithms*:

```
double sum = accumulate(s.begin(), s.end(), 0);
```

Some other STL algorithms are

- `find` finds the first element equal to the supplied value
- `count` counts the number of matching elements
- `transform` applies a supplied function to each element
- `for_each` sweeps over all elements, does not alter
- `inner_product` inner product of two vectors

Template Programming

Template programming provides a ‘language within C++’: code gets evaluated during compilation.

One of the simplest template examples is

```
template <typename T>
const T& min(const T& x, const T& y) {
    return y < x ? y : x;
}
```

This can now be used to compute the minimum between two `int` variables, or `double`, or in fact any *admissible type* providing an `operator<()` for less-than comparison.

Template Programming

Another template example is a class squaring its argument:

```
template <typename T>
class square : public std::unary_function<T,T> {
public:
    T operator()(T t) const {
        return t*t;
    }
};
```

which can be used along with STL algorithms:

```
transform(x.begin(), x.end(), square);
```

Further Reading

Books by Meyers are excellent

I also like the (free) C++ Annotations

C++ FAQ

Resources on StackOverflow such as

- general info and its links, eg
- booklist

Debugging

Debugging

Some tips:

- Generally painful, old-school `printf()` still pervasive
- Debuggers go along with compilers: `gdb` for `gcc` and `g++`; `lldb` for the clang / llvm family
- Extra tools such as `valgrind` helpful for memory debugging
- “Sanitizer” (ASAN/UBSAN) in newer versions of `g++` and `clang++`

Best Practices

Best Practices

Version control: highly recommended to become familiar with `git` or `svn`

Editor: *in the long-run*, recommended to learn productivity tricks for one editor: emacs, vi, eclipse, RStudio, ...