An Example-Driven Hands-On Introduction to Rcpp

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useR! 2014
Pre-conference Tutorial
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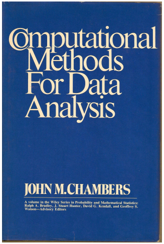
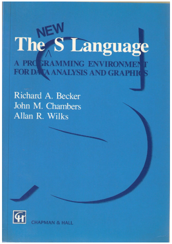
Outline

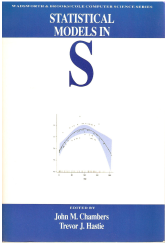
1. Why
   - R
   - C++
   - Vision
   - Features

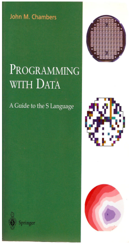
Why R?

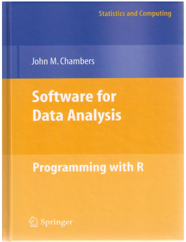
Programming with Data











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

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

Chambers and Hastie. *Statistical Models in S*. Chapman & Hall, 1992.

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

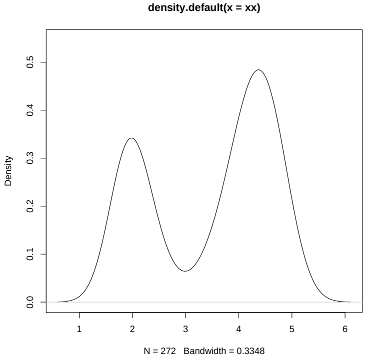
Chambers. *Software for Data Analysis: Programming with R*. Springer, 2008

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

Why R?

Succinct and expressive

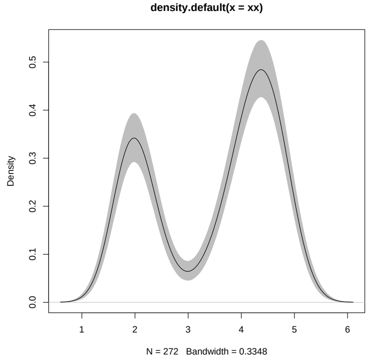
```r
xx <- faithful[,"eruptions"]
fit <- density(xx)
plot(fit)
```



Why R?

Succinct and expressive

```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)
```



The example was posted by Greg Snow on r-help a few years ago.

Why R?

Interactive

R enables us to

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

making it a preferred environment for many data analysts.

Why R?

Extensible

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 S Urbanek
- **C++** but essentially at the bare-bones level of C

So 'in theory' this worked – yet tedious 'in practice'.

Why C++?

- Asking Google [currently] leads to 64,200,000 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"*

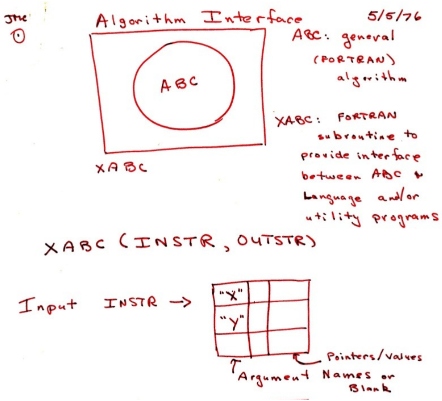
- **C** provides a rich inheritance and interoperability as Unix, Windows, ... are all build on C.
- **Object-Oriented C++** just to provide endless discussions about exactly what OO is or should be.
- **Templated C++** which is mighty powerful; template meta programming unequalled in other languages.
- **The STL** which is a specific template library which is powerful but has its own conventions.

C++11 adds enough to be called a fifth language.

Why C++?

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

Interface Vision



Source: John Chambers, personal communication.

Interface Vision

- Use trusted numerical libraries (mostly/exclusively written in Fortran)
- Provide environment which statistician could use more easily
- Enable interactive and iterative data exploration
- Make it extensibilty for research into statistical methods
- C.f. John Chambers (2008) regarding “Mission” and “Directive”

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)

Interpeted 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 it really does not have to be that complicated – we will look at a few examples

Easy to use as it avoids build and OS system complexities thanks to the R infrastrucure

Expressive 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*

Outline

2 What
- R API
- C++

What can Rcpp do?

Everything evolves around `.Call`

At the C++ level:

```
SEXP foo(SEXP a, SEXP b, SEXP C, ...)
```

and at the R level:

```
res <- .Call("foo", a, b, c, ...,
                  PACKAGE="mypkg")
```

What can Rcpp do?

Seamless interchange of R objects: C API of R

```
#include <R.h>
#include <Rdefines.h>
SEXP convolve2(SEXP a, SEXP b) {
    int i, j, na, nb, nab;
    double *xa, *xb, *xab;
    SEXP ab;

    PROTECT(a = AS_NUMERIC(a));
    PROTECT(b = AS_NUMERIC(b));
    na = LENGTH(a); nb = LENGTH(b); nab = na + nb - 1;
    PROTECT(ab = NEW_NUMERIC(nab));
    xa = NUMERIC_POINTER(a); xb = NUMERIC_POINTER(b);
    xab = NUMERIC_POINTER(ab);
    for(i = 0; i < nab; i++) xab[i] = 0.0;
    for(i = 0; i < na; i++)
        for(j = 0; j < nb; j++) xab[i + j] += xa[i] * xb[j];
    UNPROTECT(3);
    return(ab);

}
```

What can Rcpp do?

Seamless interchange of R objects: Rcpp version

```
#include <Rcpp.h>

using namespace Rcpp;

// [[Rcpp::export]]
NumericVector convolveCpp(NumericVector a, NumericVector b) {
    int na = a.size(), nb = b.size();
    int nab = na + nb - 1;
    NumericVector xab(nab);

    for (int i = 0; i < na; i++)
        for (int j = 0; j < nb; j++)
            xab[i + j] += a[i] * b[j];

    return xab;
}
```

What can Rcpp do?

Seamless interchange of R objects

- Any R object can be passed down to C++ code: vectors, matrices, list, ...
- But also functions, environments and more.
- This includes S3 and S4 objects as well as Reference Classes.
- Object attributes can be accessed directly.
- Objects can be created at the C++ level, and the R garbage collector *does the right thing* as if were an R-created object.

What can Rcpp do?

Seamless use of RNGs

```
set.seed(42); runif(5)

## [1] 0.9148 0.9371 0.2861 0.8304 0.6417

cppFunction('
NumericVector r1(int n) {
   NumericVector x(n);
   for (int i=0; i<n; i++) x[i] = R::runif(0,1);
   return(x);
}')
set.seed(42); r1(5)

## [1] 0.9148 0.9371 0.2861 0.8304 0.6417

cppFunction('NumericVector r2(int n) { return runif(n,0,1); }')
set.seed(42); r2(5)

## [1] 0.9148 0.9371 0.2861 0.8304 0.6417
```

What can Rcpp do?

Sugar: R version

```r
piR <- function(N) {
    x <- runif(N)
    y <- runif(N)
    d <- sqrt(x^2 + y^2)
    return(4 * sum(d <= 1.0) / N)
}
```

What can Rcpp do?

Sugar: C++ version

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

// [[Rcpp::export]]
double piSugar(const int N) {
    NumericVector x = runif(N);
    NumericVector y = runif(N);
    NumericVector d = sqrt(x*x + y*y);
    return 4.0 * sum(d <= 1.0) / N;
}
```

Outline

3 When
- A First Example
- A Second Example

When do we use Rcpp?

Easy speedup: An Introductory Example

Consider a function defined as

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

When do we use Rcpp?

Easy speedup: Simple R Implementation

```
fibR <- function(n) {
    if (n < 2) return(n)
    return(fibR(n-1) + fibR(n-2))
}
## Using it on first 11 arguments
sapply(0:10, fibR)

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

When do we use Rcpp?

Easy speedup: Timing R Implementation

```
benchmark(fibR(10),fibR(15),fibR(20))[,1:4]

##         test replications elapsed relative
## 1 fibR(10)          100   0.019     1.00
## 2 fibR(15)          100   0.216    11.37
## 3 fibR(20)          100   2.306   121.37
```

When do we use Rcpp?

Easy speedup: C++ Implementation

```
cppFunction("
  int fibCpp(int n) {
    if (n < 2) return(n);
    return(fibCpp(n-1) + fibCpp(n-2));
}")
## Using it on first 11 arguments
sapply(0:10, fibCpp)

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

When do we use Rcpp?

Easy speedup: Putting it all together

```
fibR <- function(n) {
    if (n<2) return(n)
    return(fibR(n-1) + fibR(n-2))
}
cppFunction('int fibCpp(int n) {
    if (n<2) return n;
    return fibCpp(n-2) + fibCpp(n-1);
}')
benchmark(fibR(25), fibCpp(25), order="relative")[,1:4]


##          test replications elapsed relative
## 2 fibCpp(25)          100   0.111      1.0
## 1   fibR(25)          100  25.633    230.9
```

When do we use Rcpp?

Easy speedup:: VAR(1) Simulation

Let's consider a simple possible VAR(1) system of k variables.

For $k = 2$:

$$X_t = X_{t-1}B + E_t$$

where X_t is a row vector of length 2, B is a 2 by 2 matrix and E_t is a row of the error matrix of 2 columns.

When do we use Rcpp?

Easy speedup:: VAR(1) Simulation

In R code, given both the coefficient and error matrices (revealing *k* and *n*):

```
rSim <- function(B,E) {
    X <- matrix(0,nrow(E), ncol(E))
    for (r in 2:nrow(E)) {
        X[r,] = X[r-1, ] %*% B + E[r, ]
    }
    return(X)
}
```

When do we use Rcpp?
Easy speedup: VAR(1) Simulation

```
cppFunction('arma::mat cppSim(arma::mat B, arma::mat E) {
    int m = E.n_rows; int n = E.n_cols;
    arma::mat X(m,n);
    X.row(0) = arma::zeros<arma::mat>(1,n);
    for (int r=1; r<m; r++) {
        X.row(r) = X.row(r-1) * B + E.row(r);
    }
    return X; }', depends="RcppArmadillo")
a <- matrix(c(0.5,0.1,0.1,0.5),nrow=2)
e <- matrix(rnorm(10000),ncol=2)
benchmark(cppSim(a,e), rSim(a,e),
          order="relative")[,1:4]

##           test replications elapsed relative
## 1 cppSim(a, e)          100   0.231     1.00
## 2   rSim(a, e)          100   2.583    11.18
```

When do we use Rcpp?

New things: Easy access to C/C++ libraries

- Sometimes speed is not the only reason
- C and C++ provide a enormous amount of libraries and APIs we may want to use
- Easy to provide access to as **Rcpp** eases data transfer to/from R
- *Rcpp modules* can make it even easier

Outline

4 Where

Where is Rcpp being used?

Numbers as of June 2014

Rcpp is

- used by 229 packages on CRAN
- used by another 27 package on BioConductor
- cited 105 times (Google Scholar count for 2011 JSS paper)

Where is Rcpp being used?

Several well-known packages

Amelia	Gary King et al: Multiple Imputation; uses **Rcpp** and **RcppArmadillo**
forecast	Rob Hyndman et al: (Automated) Time-series forecasting; uses **Rcpp** and **RcppArmadillo**
RStan	Andrew Gelman et al: Bayesian models / MCMC
rugarch	Alexios Ghalanos: Sophisticated financial models; using **Rcpp** and **RcppArmadillo**
lme4	Doug Bates et al: Hierarchical/Mixed Linear Models; uses **Rcpp** and **RcppEigen**.
dplyr, bigviz, ...	Hadley Wickham: Data munging; high-dim. visualization for 10-100 million obs.

Outline

How do we use Rcpp?

Uses only standard R tools to build packages

Depending on the platform, one needs

- **Windows** the Rtools kit for Windows, properly installed – see CRAN, the Installation manual and many tutorials; the **installr** package may help
- **OS X** the Xcode *command-line tools* (plus possibly the Fortran compiler) – see Simon's pages
- **Linux** generally just work out of the box

Several environments can be used to work with **Rcpp** – RStudio is very popular.

No additional requirements for Rcpp beyond *being able to compile R packages*.

How do we use Rcpp?

Easy to test

```
## evaluate a C++ expression, retrieve result
evalCpp("2 + 2")

## [1] 4

## a little fancier
evalCpp("std::numeric_limits<double>::max()")

## [1] 1.798e+308

## create ad-hoc R function 'square'
cppFunction('int square(int x) { return x*x;}')
square(7L)

## [1] 49
```

How do we use Rcpp?

Basic Usage: evalCpp

`evalCpp()` evaluates a single C++ expression. Includes and dependencies can be declared.

This allows us to quickly check C++ constructs.

```
evalCpp("2 * M_PI")

## [1] 6.283
```

How do we use Rcpp?

Basic Usage: `cppFunction()`

`cppFunction()` creates, compiles and links a C++ file, and creates an R function to access it.

```
cppFunction("
    int useCpp11() {
        auto x = 10;
        return x;
}", plugins=c("cpp11"))
useCpp11()   # same identifier as C++ function

## [1] 10
```

How do we use Rcpp?

Basic Usage: `sourceCpp()`

`sourceCpp()` is the actual workhorse behind `evalCpp()` and `cppFunction()`. It is described in more detail in the package vignette Rcpp-attributes.

A key feature are the plugins and dependency options: other packages can provide a plugin to supply require compile-time parameters (cf **RcppArmadillo**, **RcppEigen**, **RcppGSL**).

We have also provided plugins for other compiler features. These allow to enable support for C++11 (and beyond), as well as for OpenMP.

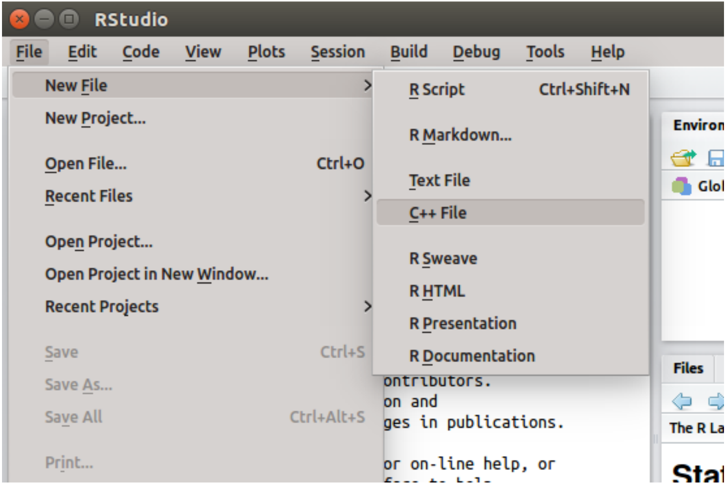
How do we use Rcpp?

Basic Usage: `Rcpp.package.skeleton()`

- To create a complete and working package, the `Rcpp.package.skeleton()` function can be used.
- It extends the base R function `package.skeleton()` and supports the same set of options.
- For **Rcpp** use is also supports (via additional options) *Rcpp Modules* and *Rcpp Attributes* both of which can be included with working examples
- The vignette Rcpp-package has complete details.

How do we use Rcpp?

RStudio makes it very easy: Single File



How do we use Rcpp?

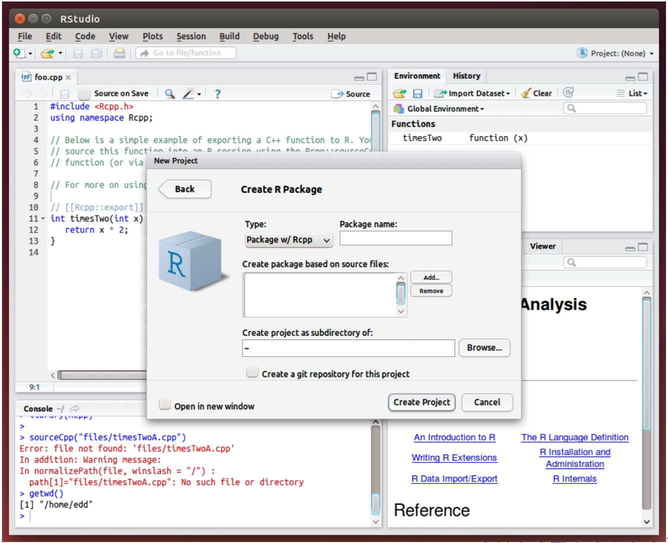
RStudio example cont'ed

The following file gets created:

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

// Below is a simple example of exporting a C++ function to R.
// You can source this function into an R session using the
// Rcpp::sourceCpp function (or via the Source button on the
// editor toolbar)

// For more on using Rcpp click the Help button on the editor
// toolbar

// [[Rcpp::export]]
int timesTwo(int x) {
   return x * 2;
}
```

How do we use Rcpp?

RStudio makes it very easy: Package



Outline

6. Examples
   - CumSum
   - R Fun
   - Boost
   - Subset
   - CtoC++
   - xts
   - XPtr

Cumulative Sum

http://gallery.rcpp.org/articles/vector-cumulative-sum/

A basic looped version:

```
#include <Rcpp.h>
#include <numeric>     // for std::partial_sum
using namespace Rcpp;

// [[Rcpp::export]]
NumericVector cumsum1(NumericVector x){
    // initialize an accumulator variable
    double acc = 0;

    // initialize the result vector
    NumericVector res(x.size());

    for(int i = 0; i < x.size(); i++){
         acc += x[i];
         res[i] = acc;
    }
    return res;
}
```

Cumulative Sum

http://gallery.rcpp.org/articles/vector-cumulative-sum/

An STL variant:

```
// [[Rcpp::export]]
NumericVector cumsum2(NumericVector x){
    // initialize the result vector
    NumericVector res(x.size());
    std::partial_sum(x.begin(), x.end(),
                     res.begin());
    return res;
}
```

Cumulative Sum

http://gallery.rcpp.org/articles/vector-cumulative-sum/

Or just **Rcpp** sugar:

```
// [[Rcpp::export]]
NumericVector cumsum3(NumericVector x){
    return cumsum(x);  // compute + return result vector

}
```

Of course, all results are the same.

```
cppFunction('NumericVector cumsum3(NumericVector x) {
                                   return cumsum(x); }')
x <- 1:10
all.equal(cumsum(x), cumsum3(x))


## [1] TRUE
```

Calling an R function from C++

http://gallery.rcpp.org/articles/r-function-from-c++/

```
#include <Rcpp.h>

using namespace Rcpp;

// [[Rcpp::export]]
NumericVector callFunction(NumericVector x,
                           Function f) {
    NumericVector res = f(x);
    return res;
}

/*** R
callFunction(x, fivenum)
*/
```

Using Boost via BH: Greatest Common Denominator

http://gallery.rcpp.org/articles/a-first-boost-example/

```
// [[Rcpp::depends(BH)]]
#include <Rcpp.h>
#include <boost/math/common_factor.hpp>

// [[Rcpp::export]]
int computeGCD(int a, int b) {
    return boost::math::gcd(a, b);
}

// [[Rcpp::export]]
int computeLCM(int a, int b) {
    return boost::math::lcm(a, b);
}
```

Using Boost via BH: Lexical Cast

http://gallery.rcpp.org/articles/a-second-boost-example/

```
// [[Rcpp::depends(BH)]]
#include <Rcpp.h>
#include <boost/lexical_cast.hpp>
using boost::lexical_cast;
using boost::bad_lexical_cast;

// [[Rcpp::export]]
std::vector<double> lexicalCast(std::vector<std::string> v) {
    std::vector<double> res(v.size());
    for (int i=0; i<v.size(); i++) {
        try {
            res[i] = lexical_cast<double>(v[i]);
        } catch(bad_lexical_cast &) {
            res[i] = NA_REAL;
        }
    }
    return res;
}
// R> lexicalCast(c("1.23", ".4", "1000", "foo", "42", "pi/4")(
// [1]    1.23    0.40 1000.00      NA   42.00       NA
```

Using Boost via BH: Date Calculations

http://gallery.rcpp.org/articles/using-boost-with-bh/

```
// [[Rcpp::depends(BH)]]
#include <Rcpp.h>

// One include file from Boost
#include <boost/date_time/gregorian/gregorian_types.hpp>

using namespace boost::gregorian;

// [[Rcpp::export]]
Rcpp::Date getIMMDate(int mon, int year) {
    // compute third Wednesday of given month / year
    date d = nth_day_of_the_week_in_month(
                   nth_day_of_the_week_in_month::third,
                   Wednesday, mon).get_date(year);
    date::ymd_type ymd = d.year_month_day();
    return Rcpp::Date(ymd.year, ymd.month, ymd.day);
}
```

Using Boost via BH: FOREACH

http://gallery.rcpp.org/articles/boost-foreach/

```
#include <Rcpp.h>
#include <boost/foreach.hpp>
using namespace Rcpp;
// [[Rcpp::depends(BH)]]

// the C-style upper-case macro name is a bit ugly
#define foreach BOOST_FOREACH

// [[Rcpp::export]]
NumericVector square( NumericVector x ) {

  // elem is a reference to each element in x
  // we can re-assign to these elements as well
  foreach( double& elem, x ) {
    elem = elem*elem;
  }
  return x;

}
```

C++11 now has something similar in a smarter `for` loop.

Using Boost via BH: Regular Expressions

http://gallery.rcpp.org/articles/boost-regular-expressions/

NB: Needs `Sys.setenv("PKG_LIBS"="-lboost_regex")` to link.

```
//
boost.org/doc/libs/1_53_0/libs/regex/example/snippets/credit_card_exam
#include <Rcpp.h>
#include <string>
#include <boost/regex.hpp>

bool validate_card_format(const std::string& s) {
    static const boost::regex e("(\\d{4}[- ]){3}\\d{4}");
    return boost::regex_match(s, e);
}

// [[Rcpp::export]]
std::vector<bool> regexDemo(std::vector<std::string> s) {
    int n = s.size();
    std::vector<bool> v(n);
    for (int i=0; i<n; i++)
        v[i]  = validate_card_format(s[i]);
    return valid;

}
```

Vector Subsetting

http://gallery.rcpp.org/articles/subsetting/

New / improved in **Rcpp** 0.11.1:

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

// [[Rcpp::export]]
NumericVector positives(NumericVector x) {
    return x[x > 0];
}

// [[Rcpp::export]]
List first_three(List x) {
    IntegerVector idx = IntegerVector::create(0, 1, 2);
    return x[idx];
}

// [[Rcpp::export]]
List with_names(List x, CharacterVector y) {
    return x[y];

}
```

Converting C to C++: A plyr example

`http://gallery.rcpp.org/articles/plyr-c-to-rcpp/`

> *The job of* `split_indices()` *is simple: given a vector* x *of integers, it returns a list where the i-th element of the list is an integer vector containing the positions of x equal to i.*

I will spare you the C API version.

Converting C to C++: A plyr example

http://gallery.rcpp.org/articles/plyr-c-to-rcpp/

```
#include <Rcpp.h>

using namespace Rcpp;

// [[Rcpp::export]]
std::vector<std::vector<int> >
split_indices(IntegerVector x, int n = 0) {
    if (n < 0) stop("n must be a pos. int.");

    std::vector<std::vector<int> > ids(n);

    int nx = x.size();
    for (int i = 0; i < nx; ++i) {
        if (x[i] > n) {
           ids.resize(x[i]);
        }
        ids[x[i] - 1].push_back(i + 1);
    }
    return ids;

}
```

Creating xts objects in C++

http://gallery.rcpp.org/articles/creating-xts-from-c++/

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

NumericVector createXts(int sv, int ev) {
    IntegerVector ind = seq(sv, ev);     // values

    NumericVector dv(ind);               // date(time)s == reals
    dv = dv * 86400;                     // scaled to days
    dv.attr("tzone")    = "UTC";         // index has attributes
    dv.attr("tclass")   = "Date";

    NumericVector xv(ind);               // data has same index
    xv.attr("dim")         = IntegerVector::create(ev-sv+1,1);
    xv.attr("index")       = dv;
    CharacterVector cls = CharacterVector::create("xts","zoo");
    xv.attr("class")       = cls;
    xv.attr(".indexCLASS") = "Date";
    // ... some more attributes ...

    return xv;
}
```

Function Pointers

http://gallery.rcpp.org/articles/passing-cpp-function-

Consider two simple functions modifying a given Armadillo vector:

```
// [[Rcpp::depends(RcppArmadillo)]]
#include <RcppArmadillo.h>

using namespace arma;
using namespace Rcpp;

vec fun1_cpp(const vec& x) { // a first function
    vec y = x + x;
    return (y);
}

vec fun2_cpp(const vec& x) { // and a second function
    vec y = 10*x;
    return (y);
}
```

Function Pointers

http://gallery.rcpp.org/articles/passing-cpp-function-

Using a `typedef` to declare an interface to a function taking and returning a vector — and a function returning a function pointer given a string argument

```
typedef vec (*funcPtr)(const vec& x);

// [[Rcpp::export]]
XPtr<funcPtr> putFunPtrInXPtr(std::string fstr) {
    if (fstr == "fun1")
        return(XPtr<funcPtr>(new funcPtr(&fun1_cpp)));
    else if (fstr == "fun2")
        return(XPtr<funcPtr>(new funcPtr(&fun2_cpp)));
    else
        // runtime err.: NULL no XPtr
        return XPtr<funcPtr>(R_NilValue);

}
```

Function Pointers

http://gallery.rcpp.org/articles/passing-cpp-function-

We then create a function calling the supplied function on a given vector by 'unpacking' the function pointer:

```
// [[Rcpp::export]]
vec callViaXPtr(const vec x, SEXP xpsexp) {
    XPtr<funcPtr> xpfun(xpsexp);
    funcPtr fun = *xpfun;
    vec y = fun(x);
    return (y);
}
```

Function Pointers

http://gallery.rcpp.org/articles/passing-cpp-function-

```
## get us a function
fun <- putFunPtrInXPtr("fun1")
## and pass it down to C++ to
## have it applied on given vector
callViaXPtr(1:4, fun)

##      [,1]
## [1,]    2
## [2,]    4
## [3,]    6
## [4,]    8
```

Could use same mechanism for user-supplied functions, gradients, or samplers, ...

Outline

Armadillo

Armadillo: C++ linear algebra library - Google Chrome

Armadillo: C++ linear alge ×

arma.sourceforge.net

Armadillo

C++ linear algebra library

NICTA

About License FAQ API Docs Speed Authors Download

- Armadillo is a C++ linear algebra library (matrix maths) aiming towards a good balance between speed and ease of use
- The syntax (API) is deliberately similar to Matlab
- Integer, floating point and complex numbers are supported, as well as a subset of trigonometric and statistics functions
- Various matrix decompositions are provided through optional integration with LAPACK, or one of its high performance drop-in replacements (such as the multi-threaded Intel MKL, or AMD ACML, or OpenBLAS libraries)
- A delayed evaluation approach is employed (at compile-time) to combine several operations into one and reduce (or eliminate) the need for temporaries; this is automatically accomplished through template meta-programming
- Useful for conversion of research code into production environments, or if C++ has been decided as the language of choice, due to speed and/or integration capabilities
- The library is open-source software, and is distributed under a license that is useful in both open-source and commercial/proprietary contexts
- Primarily developed at NICTA (Australia) by Conrad Sanderson, with contributions from around the world
- **Download latest version**

What is Armadillo?

From `arma.sf.net` and slightly edited

- Armadillo is a C++ linear algebra library (matrix maths) aiming towards a good balance between speed and ease of use.
- The syntax is deliberately similar to Matlab.
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What is Armadillo?

From `arma.sf.net` and slightly edited

- Armadillo is a C++ linear algebra library (matrix maths) aiming towards a good balance between **speed and ease of use.**
- The syntax is **deliberately similar to Matlab.**
- **Integer, floating point and complex numbers** are supported.
- A **delayed evaluation approach** is employed (at compile-time) to combine several operations into one and reduce (or eliminate) the need for temporaries.
- Useful for conversion of research code into **production environments**, or if C++ has been decided as the language of choice, due to **speed** and/or integration capabilities.

Armadillo highlights

- Provides integer, floating point and complex vectors, matrices and fields (3d) with all the common operations.
- Very good documentation and examples at website `http://arma.sf.net`, a technical report (Sanderson, 2010)
- Modern code, building upon and extending from earlier matrix libraries.
- Responsive and active maintainer, frequent updates.
- Used by MLPACK; cf Curtin et al (JMLR, 2013)

RcppArmadillo highlights

- Template-only builds—no linking, and available whereever R and a compiler work (but **Rcpp** is needed)!
- Easy with R packages: just add `LinkingTo: RcppArmadillo, Rcpp` to DESCRIPTION (*i.e.*, no added cost beyond **Rcpp**)
- Data exchange really seamless from R via **Rcpp**
- Frequently updated; documentation includes Eddelbuettel and Sanderson (CSDA, 2014).

Well-know packages using RcppArmadillo

Amelia by Gary King et al: Multiple Imputation from cross-section, time-series or both;

forecast by Rob Hyndman et al: Time-series forecasting including state space and automated ARIMA modeling;

rugarch by Alexios Ghalanos: Sophisticated financial time series models;

gRbase by Søren Højsgaard: Graphical modeling

Armadillo Eigenvalues

http://gallery.rcpp.org/articles/armadillo-eigenvalues/

```
#include <RcppArmadillo.h>

// [[Rcpp::depends(RcppArmadillo)]]

// [[Rcpp::export]]
arma::vec getEigenValues(arma::mat M) {
    return arma::eig_sym(M);
}
```

Armadillo Eigenvalues

http://gallery.rcpp.org/articles/armadillo-eigenvalues/

```
set.seed(42); X <- matrix(rnorm(4*4), 4, 4)
Z <- X %*% t(X); getEigenValues(Z)

##            [,1]
## [1,]   0.3319
## [2,]   1.6856
## [3,]   2.4099
## [4,] 14.2100

# R gets the same results (in reverse)
# and also returns the eigenvectors.
```

Multivariate Normal RNG Draw

http://gallery.rcpp.org/articles/simulate-multivariate-norn

```
#include <RcppArmadillo.h>
// [[Rcpp::depends(RcppArmadillo)]]

// [[Rcpp::export]]
arma::mat mvrnormArma(int n, arma::vec mu,
                      arma::mat sigma) {
   arma::mat Y = arma::randn(n, sigma.n_cols);
   return arma::repmat(mu, 1, n).t() +
                  Y * arma::chol(sigma);
}
```

Faster Linear Model with FastLm
Background

- Implementations of ‘fastLm()‘ have been a staple all along the development of **Rcpp**
- The very first version was in response to a question by Ivo Welch on r-help.
- The request was for a fast function to estimate parameters – and their standard errors – from a linear model,
- It used GSL functions to estimate $\hat{\beta}$ as well as its standard errors $\hat{\sigma}$ – as `lm.fit()` in R only returns the former.
- It had since been reimplemented for **RcppArmadillo** and **RcppEigen**.

Faster Linear Model with FastLm

Initial RcppArmadillo src/fastLm.cpp

```
#include <RcppArmadillo.h>

extern "C" SEXP fastLm(SEXP Xs, SEXP ys) {

  try {
    Rcpp::NumericVector yr(ys);                 // creates Rcpp vector from SEXP
    Rcpp::NumericMatrix Xr(Xs);                 // creates Rcpp matrix from SEXP
    int n = Xr.nrow(), k = Xr.ncol();
    arma::mat X(Xr.begin(), n, k, false);       // reuses memory, avoids extra
copy
    arma::colvec y(yr.begin(), yr.size(), false);

    arma::colvec coef = arma::solve(X, y);      // fit model y ∼ X
    arma::colvec res  = y - X*coef;             // residuals
    double s2 = std::inner_product(res.begin(), res.end(), res.begin(), 0.0)/(n - k);
    arma::colvec std_err =                      // std.errors of coefficients
        arma::sqrt(s2*arma::diagvec(arma::pinv(arma::trans(X)*X)));

    return Rcpp::List::create(Rcpp::Named("coefficients") = coef,
                              Rcpp::Named("stderr")       = std_err,
                              Rcpp::Named("df.residual")  = n - k    );
  } catch( std::exception &ex ) {
    forward_exception_to_r( ex );
  } catch(...) {
    ::Rf_error( "c++ exception (unknown reason)" );
  }
  return R_NilValue; // -Wall

}
```

Faster Linear Model with FastLm

Edited version of earlier RcppArmadillo's `src/fastLm.cpp`

```
// [[Rcpp::depends(RcppArmadillo)]]
#include <RcppArmadillo.h>
using namespace Rcpp; using namespace arma;

// [[Rcpp::export]]
List fastLm(NumericVector yr, NumericMatrix Xr) {
   int n = Xr.nrow(), k = Xr.ncol();
   mat X(Xr.begin(), n, k, false);
   colvec y(yr.begin(), yr.size(), false);

   colvec coef = solve(X, y);
   colvec resid = y - X*coef;

   double sig2 = as_scalar(trans(resid)*resid/(n-k));
   colvec stderrest = sqrt(sig2 * diagvec( inv(trans(X)*X)) );

   return List::create(Named("coefficients") = coef,
                       Named("stderr")       = stderrest,
                       Named("df.residual")  = n - k    );
}
```

Faster Linear Model with FastLm

Current version of RcppArmadillo's src/fastLm.cpp

```
// [[Rcpp::depends(RcppArmadillo)]]
#include <RcppArmadillo.h>
using namespace Rcpp;
using namespace arma;

// [[Rcpp::export]]
List fastLm(const arma::mat& X, const arma::colvec& y) {
   int n = X.n_rows, k = X.n_cols;

   colvec coef = solve(X, y);
   colvec resid = y - X*coef;

   double sig2 = as_scalar(trans(resid)*resid/(n-k));
   colvec stderrest = sqrt(sig2 * diagvec( inv(trans(X)*X)) );

   return List::create(Named("coefficients") = coef,
                       Named("stderr")       = stderrest,
                       Named("df.residual")  = n - k    );

}
```

Faster Linear Model with FastLm

Note on as<>() casting with Armadillo

```
arma::colvec y = Rcpp::as<arma::colvec>(ys);

arma::mat X = Rcpp::as<arma::mat>(Xs);
```

Convenient, yet incurs an additional copy. Next variant uses two steps, but only a pointer to objects is copied:

```
Rcpp::NumericVector yr(ys);
Rcpp::NumericMatrix Xr(Xs);
int n = Xr.nrow(), k = Xr.ncol();
arma::mat X(Xr.begin(), n, k, false);

arma::colvec y(yr.begin(), yr.size(), false);
```

Preferable if performance is a concern. Since last fall **RcppArmadillo** has efficient `const references` too.

Faster Linear Model with FastLm
Performance comparison

Running the script included in the **RcppArmadillo** package:

```
edd@max:~/svn/rcpp/pkg/RcppArmadillo/inst/examples$ r fastLm.r
Loading required package: Rcpp
                       test replications relative elapsed
2          fLmTwoCasts(X, y)         5000    1.000   0.188
3          fLmConstRef(X, y)         5000    1.000   0.188
1           fLmOneCast(X, y)         5000    1.005   0.189
5    fastLmPureDotCall(X, y)         5000    1.064   0.200
4           fastLmPure(X, y)         5000    2.000   0.376
7               lm.fit(X, y)         5000    2.691   0.506
6 fastLm(frm, data = trees)         5000   35.596   6.692
8     lm(frm, data = trees)         5000   44.883   8.438
edd@max:~/svn/rcpp/pkg/RcppArmadillo/inst/examples$
```

Kalman Filter

Setup at Mathworks site

The position of an object is estimated based on past values of 6×1 state vectors X and Y for position, V_X and V_Y for speed, and A_X and A_Y for acceleration.

Position updates as a function of the speed

$$X = X_0 + V_X dt \qquad \text{and} \qquad Y = Y_0 + V_Y dt,$$

which is updated as a function of the (unobserved) acceleration:

$$V_x = V_{X,0} + A_X dt \qquad \text{and} \qquad V_y = V_{Y,0} + A_Y dt.$$

Kalman Filter

Basic Matlab Function

```
% Copyright 2010 The MathWorks, Inc.
function y = kalmanfilter(z)
% #codegen
    dt=1;
    % Initialize state transition matrix
    A=[1 0 dt 0 0 0;...       % [x  ]
       0 1 0 dt 0 0;...       % [y  ]
       0 0 1 0 dt 0;...       % [Vx]
       0 0 0 1 0 dt;...       % [Vy]
       0 0 0 0 1 0 ;...       % [Ax]
       0 0 0 0 0 1 ];         % [Ay]
    H = [ 1 0 0 0 0 0; 0 1 0 0 0 0 ];
    Q = eye(6);
    R = 1000 * eye(2);
    persistent x_est p_est
    if isempty(x_est)
        x_est = zeros(6, 1);
        p_est = zeros(6, 6);
    end
```

```
    % Predicted state and covariance
    x_prd = A * x_est;
    p_prd = A * p_est * A' + Q;
    % Estimation
    S = H * p_prd' * H' + R;
    B = H * p_prd';
    klm_gain = (S \ B)';
    % Estimated state and covariance
    x_est = x_prd+klm_gain*(z-H*x_prd);
    p_est = p_prd-klm_gain*H*p_prd;
    % Compute the estimated measurements
    y = H * x_est;
end                    % of the function
```

Plus a simple wrapper function calling this function.

Kalman Filter: In R

Easy enough – first naive solution

```r
FirstKalmanR <- function(pos) {

  kf <- function(z) {
    dt <- 1

    A <- matrix(c(1, 0, dt, 0, 0, 0,   # x
                  0, 1, 0, dt, 0, 0,   # y
                  0, 0, 1, 0, dt, 0,   # Vx
                  0, 0, 0, 1, 0, dt,   # Vy
                  0, 0, 0, 0, 1,  0,   # Ax
                  0, 0, 0, 0, 0,  1),  # Ay
                6, 6, byrow=TRUE)
    H <- matrix( c(1, 0, 0, 0, 0, 0,
                   0, 1, 0, 0, 0, 0),
                2, 6, byrow=TRUE)
    Q <- diag(6)
    R <- 1000 * diag(2)

    N <- nrow(pos)
    y <- matrix(NA, N, 2)

    ## predicted state and covriance
    xprd <- A %*% xest
    pprd <- A %*% pest %*% t(A) + Q

    ## estimation
    S <- H %*% t(pprd) %*% t(H) + R
    B <- H %*% t(pprd)
    ##  kalmangain <- (S \ B)'
    kg <- t(solve(S, B))

    ## est. state and cov, assign to vars
in parent env
    xest <<- xprd + kg %*% (z-H%*%xprd)
    pest <<- pprd - kg %*% H %*% pprd

    ## compute the estimated measurements
    y <- H %*% xest
  }

  xest <- matrix(0, 6, 1)
  pest <- matrix(0, 6, 6)

  for (i in 1:N) {
      y[i,] <- kf(t(pos[i,,drop=FALSE]))
  }

  invisible(y)
}
```

Kalman Filter: In R

Easy enough – with some minor refactoring

```r
KalmanR <- function(pos) {

  kf <- function(z) {
    ## predicted state and covriance
    xprd <- A %*% xest
    pprd <- A %*% pest %*% t(A) + Q

    ## estimation
    S <- H %*% t(pprd) %*% t(H) + R
    B <- H %*% t(pprd)
    ##  kg <- (S \ B)'
    kg <- t(solve(S, B))

    ## estimated state and covariance
    ## assigned to vars in parent env
    xest <<- xprd + kg %*% (z-H%*%xprd)
    pest <<- pprd - kg %*% H %*% pprd

    ## compute the estimated measurements
    y <- H %*% xest
  }
  dt <- 1
  A <- matrix(c(1, 0, dt, 0, 0, 0, # x
                0, 1, 0, dt, 0, 0, # y
                0, 0, 1, 0, dt, 0, # Vx
                0, 0, 0, 1, 0, dt, # Vy
                0, 0, 0, 0, 1,  0, # Ax
                0, 0, 0, 0, 0,  1),# Ay
                6, 6, byrow=TRUE)
  H <- matrix(c(1, 0, 0, 0, 0, 0,
                0, 1, 0, 0, 0, 0),
              2, 6, byrow=TRUE)
  Q <- diag(6)
  R <- 1000 * diag(2)

  N <- nrow(pos)
  y <- matrix(NA, N, 2)

  xest <- matrix(0, 6, 1)
  pest <- matrix(0, 6, 6)

  for (i in 1:N) {
    y[i,] <- kf(t(pos[i,,drop=FALSE]))
  }
  invisible(y)
}
```

Kalman Filter: In C++

Using a simple class

```cpp
// [[Rcpp::depends(RcppArmadillo)]]
#include <RcppArmadillo.h>

using namespace arma;

class Kalman {
private:
  mat A, H, Q, R, xest, pest;
  double dt;

public:
  // constructor, sets up data structures
  Kalman() : dt(1.0) {
    A.eye(6,6);
    A(0,2) = A(1,3) = dt;
    A(2,4) = A(3,5) = dt;
    H.zeros(2,6);
    H(0,0) = H(1,1) = 1.0;
    Q.eye(6,6);
    R = 1000 * eye(2,2);
    xest.zeros(6,1);
    pest.zeros(6,6);

  }
```

```cpp
// sole member func.: estimate model
mat estimate(const mat & Z) {
  unsigned int n = Z.n_rows,
               k = Z.n_cols;
  mat Y = zeros(n, k);
  mat xprd, pprd, S, B, kg;
  colvec z, y;

  for (unsigned int i = 0; i<n; i++) {
    z = Z.row(i).t();
    // predicted state and covariance
    xprd = A * xest;
    pprd = A * pest * A.t() + Q;
    // estimation
    S = H * pprd.t() * H.t() + R;
    B = H * pprd.t();
    kg = (solve(S, B)).t();
    // estimated state and covariance
    xest = xprd + kg * (z - H * xprd);
    pest = pprd - kg * H * pprd;
    // compute estimated measurements
    y = H * xest;
    Y.row(i) = y.t();
  }
  return Y;
}
```

Kalman Filter in C++

Trivial to use from R

Given the code from the previous slide, we just add

```
// [[Rcpp::export]]
mat KalmanCpp(mat Z) {
  Kalman K;
  mat Y = K.estimate(Z);
  return Y;
}
```

Kalman Filter: Performance

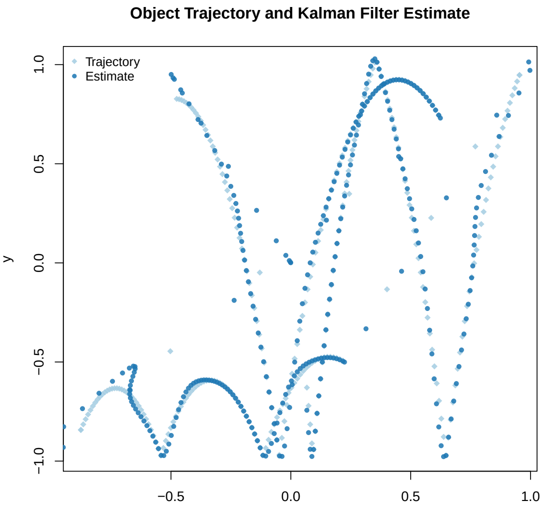
Quite satisfactory relative to R

Even byte-compiled 'better' R version is 66 times slower:

```
R> FirstKalmanRC <- cmpfun(FirstKalmanR)
R> KalmanRC <- cmpfun(KalmanR)
R>
R> stopifnot(identical(KalmanR(pos), KalmanRC(pos)),
+            all.equal(KalmanR(pos), KalmanCpp(pos)),
+            identical(FirstKalmanR(pos), FirstKalmanRC(pos)),
+            all.equal(KalmanR(pos), FirstKalmanR(pos)))
R>
R> res <- benchmark(KalmanR(pos), KalmanRC(pos),
+                  FirstKalmanR(pos), FirstKalmanRC(pos),
+                  KalmanCpp(pos),
+                  columns = c("test", "replications",
+                              "elapsed", "relative"),
+                  order="relative",
+                  replications=100)
R>
R> print(res)
                test replications elapsed relative
5     KalmanCpp(pos)          100   0.087   1.0000
2      KalmanRC(pos)          100   5.774  66.3678
1       KalmanR(pos)          100   6.448  74.1149
4 FirstKalmanRC(pos)          100   8.153  93.7126
3  FirstKalmanR(pos)          100   8.901 102.3103
```

Kalman Filter: Figure

Last but not least we can redo the plot as well



Sparse Matrices

Growing (but incomplete) support in Armadillo

A nice example for work on R objects.

```
i <- c(1,3:8)
j <- c(2,9,6:10)
x <- 7 * (1:7)
A <- sparseMatrix(i, j, x = x)
A
```

```
## 8 x 10 sparse Matrix of class "dgCMatrix"
##
## [1,] . 7 . . .  .  .  .  .  .
## [2,] . . . . .  .  .  .  .  .
## [3,] . . . . .  .  .  . 14  .
## [4,] . . . . . 21  .  .  .  .
## [5,] . . . . .  . 28  .  .  .
## [6,] . . . . .  .  . 35  .  .
## [7,] . . . . .  .  .  . 42  .
## [8,] . . . . .  .  .  .  . 49
```

Sparse Matrices

Representation in R

```
str(A)

## Formal class 'dgCMatrix' [package "Matrix"] with 6 slots
##   ..@ i        : int [1:7] 0 3 4 5 2 6 7
##   ..@ p        : int [1:11] 0 0 1 1 1 1 2 3 4 6 ...
##   ..@ Dim      : int [1:2] 8 10
##   ..@ Dimnames:List of 2
##   .. ..$ : NULL
##   .. ..$ : NULL
##   ..@ x        : num [1:7] 7 21 28 35 14 42 49
##   ..@ factors : list()
```

Note how the construction was in terms of $< i, j, x >$, yet the representation in in terms of $< i, p, x >$ – CSC format.

Sparse Matrices
C++ access

```
#include <RcppArmadillo.h>

using namespace Rcpp;
using namespace arma;

// [[Rcpp::depends(RcppArmadillo)]]

// [[Rcpp::export]]
sp_mat armaEx(S4 mat, bool show) {
    IntegerVector dims = mat.slot("Dim");
    arma::urowvec i = Rcpp::as<arma::urowvec>(mat.slot("i"));
    arma::urowvec p = Rcpp::as<arma::urowvec>(mat.slot("p"));
    arma::vec x     = Rcpp::as<arma::vec>(mat.slot("x"));

    int nrow = dims[0], ncol = dims[1];
    arma::sp_mat res(i, p, x, nrow, ncol);
    if (show) Rcpp::Rcout << res << std::endl;
    return res;
}
```

Sparse Matrices

C++ access

```
sourceCpp('code/sparseEx.cpp')
i <- c(1,3:8)
j <- c(2,9,6:10)
x <- 7 * (1:7)
A <- sparseMatrix(i, j, x = x)
B <- armaEx(A, TRUE)


## [matrix size: 8x10; n_nonzero: 7; density: 8.75%]
##
##      (0, 1)          7.0000
##      (3, 5)         21.0000
##      (4, 6)         28.0000
##      (5, 7)         35.0000
##      (2, 8)         14.0000
##      (6, 8)         42.0000
##      (7, 9)         49.0000
```

Outline

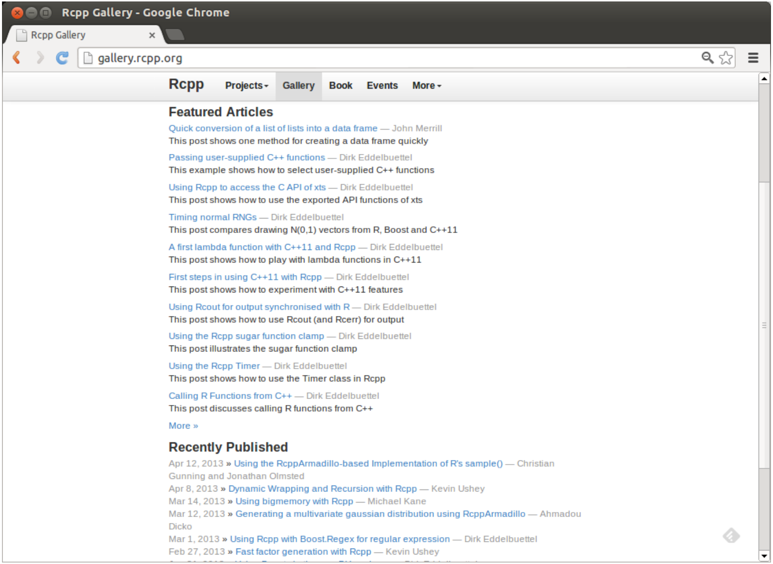
What Else?

Basic Documentation

- The package comes with **eight pdf vignettes**, and numerous help pages.
- The introductory vignettes are now **published** (Rcpp and RcppEigen in *J Stat Software*, RcppArmadillo in *Comp. Stat.& Data Anal.*).
- The **rcpp-devel** list is *the* recommended resource, generally very helpful, and fairly low volume.
- **StackOverflow** has over 500 posts too.
- Several blog posts introduce/discuss features.

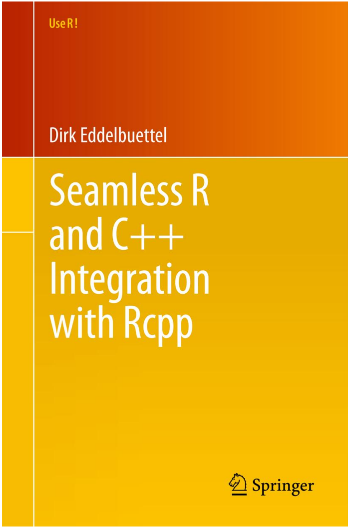
What Else?

Rcpp Gallery: 80+ working and detailed examples



What Else?

The Rcpp book



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