Seamless R Extensions using Rcpp and RInside

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Debian & R

Joint work with Romain François

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UCLA Department of Statistics (3pm)
Los Angeles R Users Group (6pm)
Outline

1. Extending R
   - Why?
     - The standard API
     - Inline

2. Rcpp
   - Overview
   - New API
   - Examples

3. Rcpp Usage Examples
   - RInside
   - Others

4. Summary
   - Key points
   - Resources
Chambers (2008) opens chapter 11 (*Interfaces I: Using C and Fortran*) with these words:

> 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.
Chambers (2008) then 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

So is the deck stacked against us?
R offers several functions to access compiled code: we focus on `.C` and `.Call` here. *(R Extensions*, sections 5.2 and 5.9; *Software for Data Analysis*).

The canonical example is the convolution function:

```c
void convolve(double *a, int *na, double *b, 
               int *nb, double *ab)
{
    int i, j, nab = *na + *nb - 1;

    for(i = 0; i < nab; i++)
        ab[i] = 0.0;

    for(i = 0; i < *na; i++)
        for(j = 0; j < *nb; j++)
            ab[i + j] += a[i] * b[j];
}
```

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Seamless R Extensions using Rcpp + RInside
The convolution function is called from R by

```r
cov <- function(a, b)
  .C("convolve",
     as.double(a),
     as.integer(length(a)),
     as.double(b),
     as.integer(length(b)),
     ab = double(length(a) + length(b) - 1))$ab
```

As stated in the manual, one must take care to coerce all the arguments to the correct R storage mode before calling `.C` as mistakes in matching the types can lead to wrong results or hard-to-catch errors.
Using `.Call`, the example becomes

```c
#include <R.h>
#include <Rdefines.h>

extern "C" 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);
}
```
Now the call simplifies to just the function name and the vector arguments—all other handling is done at the C/C++ level:

```
conv <- function(a, b) .Call("convolve2", a, b)
```

In summary, we see that

- there are different entry points
- using different calling conventions
- leading to code that may need to do more work at the lower level.
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inline is a package by Oleg Sklyar et al that provides the function `cfunction` which can wrap Fortran, C or C++ code.

```r
## A simple Fortran example
code <- "
   integer i
   do 1 i=1, n(1)
      1 x(i) = x(i)**3
"
cubefn <- cfunction(signature(n="integer", x="numeric"),
                  code, convention=".Fortran")
x <- as.numeric(1:10)
n <- as.integer(10)
cubefn(n, x)$x
```

cfunction takes care of compiling, linking, loading, ... by placing the resulting dynamically-loadable object code in the per-session temporary directory used by R.
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Compiled Code: Rcpp

In a nutshell:

- **Rcpp** makes it easier to interface C++ and **R** code.
- Using the `.Call` interface, we can use features of the C++ language to automate the tedious bits of the macro-based C-level interface to **R**.
- One major advantage of using `.Call` is that richer **R** objects (vectors, matrices, lists, ... in fact most SEXP types incl functions, environments etc) can be passed directly between **R** and C++ without the need for explicit passing of dimension arguments.
- By using the C++ class layers, we do not need to manipulate the SEXP objects using any of the old-school C macros.
- **inline** eases usage, development and testing.
The convolution example can be rewritten in the ’Classic API’:

```cpp
#include <Rcpp.h>

RcppExport SEXP convolve_cpp(SEXP a, SEXP b)
{
    RcppVector<double> xa(a);
    RcppVector<double> xb(b);

    int nab = xa.size() + xb.size() - 1;

    RcppVector<double> xab(nab);
    for (int i = 0; i < nab; i++) xab(i) = 0.0;

    for (int i = 0; i < xa.size(); i++)
        for (int j = 0; j < xb.size(); j++)
            xab(i + j) += xa(i) * xb(j);

    RcppResultSet rs;
    rs.add("ab", xab);
    return rs.getReturnList();
}
```
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Rcpp was significantly extended over the last few months to permit more natural expressions. Consider this comparison between the R API and the new Rcpp API:

```
SEXP ab;
PROTECT(ab = allocVector(STRSXP, 2));
SET_STRING_ELT(ab, 0, mkChar("foo"));
SET_STRING_ELT(ab, 1, mkChar("bar"));
UNPROTECT(1);
```

```
CharacterVector ab(2);
ap[0] = "foo";
ap[1] = "bar";
```

Data types, including STL containers and iterators, can be nested and other niceties. Implicit converters allow us to combine types:

```
std::vector<double> vec;
[...]
List x(3);
x[0] = vec;
x[1] = "some text";
x[2] = 42;
```

```
// With Rcpp 0.7.11 or later we can do:
std::vector<double> vec;
[...]
List x = List::create(vec,
          "some text",
          42);
```
Functional programming in both languages

In R, functional programming is easy:

```
R> data(faithful); lapply(faithful, summary)
$eruptions
  Min. 1st Qu.  Median    Mean  3rd Qu.    Max.  
  1.60    2.16    4.00    3.49     4.45     5.10

$waiting
  Min. 1st Qu.  Median    Mean  3rd Qu.    Max.  
  43.0    58.0    76.0    70.9     82.0     96.0
```

We can do that in C++ as well and pass the R function down to the data elements we let the STL iterate over:

```
src <- 'Rcpp::List input(data);
    Rcpp::Function f(fun);
    Rcpp::List output(input.size());
    std::transform(input.begin(), input.end(), output.begin(), f);
    output.names() = input.names();
    return output;
'cpp_lapply <- cfunction(signature(data="list", fun = "function"), src, Rcpp = TRUE )
```
Exception handling

Automatic catching and conversion of C++ exceptions:

R> library(Rcpp); library(inline)
R> cpp <- '  
+ Rcpp::NumericVector x(xs); // automatic conversion from SEXP
+ for (int i=0; i<x.size(); i++) {
+     if (x[i] < 0)
+         throw std::range_error("Non-negative values required");
+     x[i] = log(x[i]);
+ }
+ return x; // automatic conversion to SEXP
+ '
R> fun <- cfunction(signature(xs="numeric"), cpp, Rcpp=TRUE)
R> fun( seq(2, 5) )
   [1] 0.6931 1.0986 1.3863 1.6094
R> fun( seq(5, -2) )
Error in fun(seq(5, -2)) : Non-negative values required
R> fun( LETTERS[1:5] )
Error in fun(LETTERS[1:5]) : not compatible with INTSXP
R>
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The convolution example can be rewritten in the new API:

```cpp
#include <Rcpp.h>

RcppExport SEXP convolve_cpp(SEXP a, SEXP b) {
    Rcpp::NumericVector xa(a);  // automatic conversion from SEXP
    Rcpp::NumericVector xb(b);

    int n_xa = xa.size();
    int n_xb = xb.size();
    int nab = n_xa + n_xb - 1;

    Rcpp::NumericVector xab(nab);

    for (int i = 0; i < n_xa; i++)
        for (int j = 0; j < n_xb; j++)
            xab[i + j] += xa[i] * xb[j];

    return xab;  // automatic conversion to SEXP
}
```
Speed comparison

In a recently-submitted paper, the following table summarises the performance of convolution examples:

<table>
<thead>
<tr>
<th>Implementation</th>
<th>Time in millisec</th>
<th>Relative to R API</th>
</tr>
</thead>
<tbody>
<tr>
<td>R API (as benchmark)</td>
<td>32</td>
<td>1.0</td>
</tr>
<tr>
<td>RcppVector&lt;double&gt;</td>
<td>354</td>
<td>11.1</td>
</tr>
<tr>
<td>NumericVector::operator[]</td>
<td>52</td>
<td>1.6</td>
</tr>
<tr>
<td>NumericVector::begin</td>
<td>33</td>
<td></td>
</tr>
</tbody>
</table>

Table 1: Performance for convolution example

We averaged 1000 replications with two 100-element vectors – see examples/ConvolveBenchmarks/ in Rcpp for details.
Regression is a key component of many studies. In simulations, we often want to run a very large number of regressions.

\textbf{R} has \texttt{lm()} as the general purposes function. It is very powerful and returns a rich object—but it is not \textit{lightweight}.

For this purpose, \textbf{R} has \texttt{lm.fit()}. But, this does not provide all relevant auxiliary data as \textit{e.g.} the standard error of the estimate.

For the most recent \textit{Introduction to High-Performance Computing with R} tutorial, I had written a hybrid R/C/C++ solution using the GNU GSL.

We complement this with a new C++ implementation around the Armadillo linear algebra classes.
Linear regression via GSL: `lmGSL()`

```r
lmGSL <- function() {
  src <- '

  RcppVectorView<double> Yr(Ysexp);
  RcppMatrixView<double> Xr(Xsexp);

  int i, j, n = Xr.dim1(), k = Xr.dim2();
  double chi2;

  gsl_matrix *X = gsl_matrix_alloc(n,k);
  gsl_vector *y = gsl_vector_alloc(n);
  gsl_vector *c = gsl_vector_alloc(k);
  gsl_matrix *cov = gsl_matrix_alloc(k,k);

  for (i = 0; i < n; i++) {
    for (j = 0; j < k; j++) {
      gsl_matrix_set (X, i, j, Xr(i,j));
    }
    gsl_vector_set (y, i, Yr(i));
  }

  gsl_multifit_linear_workspace *wk =
    gsl_multifit_linear_alloc(n,k);
  gsl_multifit_linear(X, y, c, cov, &chi2, wk);
  gsl_multifit_linear_free (wk);
  RcppVector<double> StdErr(k);
  RcppVector<double> Coef(k);

  for (i = 0; i < k; i++) {
    Coef(i) = gsl_vector_get(c, i);
    StdErr(i) =
      sqrt(gsl_matrix_get(cov, i, i));
  }

  gsl_matrix_free(X);
  gsl_vector_free(y);
  gsl_vector_free(c);
  gsl_matrix_free(cov);

  RcppResultSet rs;
  rs.add("coef", Coef);
  rs.add("stderr", StdErr);

  return = rs.getReturnList();
  }
```

## turn into a function that R can call
## args redundant on Debian/Ubuntu
fun <-
  cfunction(signature(Ysexp="numeric",
    Xsexp="numeric"), src,
    includes=
      "# include <gsl/gsl_multifit.h>",
    Rcpp=TRUE,
    cppargs="-I/usr/include",
    libargs="-l gsl -l gslcoreblas")
```
Extending R Rcpp Examples Summary

Overview New API Examples

Linear regression via Armadillo: lmArmadillo example

```
ImArmadillo <- function() {
  src <- 'Rcpp::NumericVector yr(Ysexp);
  Rcpp::NumericVector Xr(Xsexp); // actually an n x k matrix
  std::vector<int> dims = Xr.attr("dim");
  int n = dims[0], k = dims[1];
  arma::mat X(Xr.begin(), n, k, false); // use advanced armadillo constructors
  arma::colvec y(yr.begin(), yr.size());
  arma::colvec coef = solve(X, y); // model fit
  arma::colvec resid = y - X*coef; // to comp. std.errr of the coefficients
  arma::mat covmat = trans(resid)*resid/(n-k) * arma::inv(arma::trans(X)*X);

  Rcpp::NumericVector coefr(k), stderrrestr(k);
  for (int i=0; i<k; i++) { // with RcppArmadillo template converters
    coefr[i] = coef[i]; // this would not be needed but we only
    stderrrestr[i] = sqrt(covmat(i,i)); // have Rcpp.h here
  }

  return Rcpp::List::create( Rcpp::Named("coefficients", coefr), // Rcpp 0.7.11
    Rcpp::Named("stderr", stderrrestr));

  ## turn into a function that R can call
  fun <- cfunction(signature(Ysexp="numeric", Xsexp="numeric"),
    src, includes="#include <armadillo>", Rcpp=TRUE,
    cppargs="-I/usr/include", libargs="-larmadillo")
}
```
**Linear regression via Armadillo: RcppArmadillo**

**fastLm in the new RcppArmadillo does even better:**

```c++
#include <RcppArmadillo.h>

extern "C" SEXP fastLm(SEXP ys, SEXP Xs) {
  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 and avoids extra copy
  arma::colvec y(yr.begin(), yr.size(), false);

  arma::colvec coef = arma::solve(X, y); // fit model y ~ X
  arma::colvec resid = y - X*coef; // residuals

  double sig2 = arma::as_scalar(arma::trans(resid)*resid/(n-k)); // std.err est
  arma::colvec sdest = arma::sqrt(sig2*arma::diagvec(arma::inv(arma::trans(X)*X)));

  return Rcpp::List::create( // requires Rcpp 0.7.11
    Rcpp::Named("coefficients") = coef,
    Rcpp::Named("stderr") = sdest
  );
}
```
Rcpp Example: Regression timings

Comparison of R and linear model fit routines

The small `longley` example exhibits less variability between methods, but the larger data set shows the gains more clearly.

For the small data set, all three appear to improve similarly on `lm`.

Source: Our calculations, see examples/FastLM/ in Rcpp.
Another Rcpp example (cont.)

**Comparison of R and linear model fit routines**

By dividing the `lm` time by the respective times, we obtain the 'possible gains' from switching.

One caveat, measurements depends critically on the size of the data as well as the cpu and libraries that are used.

Source: Our calculations, see examples/FastLM/ in Rcpp.
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Jeff Horner’s work on RApache lead to joint work in littler, a scripting / cmdline front-end. As it embeds R and simply ‘feeds’ the REPL loop, the next step was to embed R in proper C++ classes: RInside.

```cpp
#include <RInside.h> // for the embedded R via RInside

int main(int argc, char *argv[]) {
  RInside R(argc, argv); // create an embedded R instance
  R["txt"] = "Hello, world!\n"; // assign a char* (string) to 'txt'
  R.parseEvalQ("cat(txt)"); // eval the init string, ignoring any returns
  exit(0);
}
```
Another simple example

This example shows some of the new assignment and converter code:

```
#include <RInside.h>       // for the embedded R via RInside

int main(int argc, char *argv[]) {
    RInside R(argc, argv); // create an embedded R instance

    R["x"] = 10;
    R["y"] = 20;

    R.parseEvalQ("z <- x + y");

    int sum = R["z"];

    std::cout << "10 + 20 = " << sum << std::endl;
    exit(0);
}
```
And another parallel example

```c++
#include <mpi.h>    // mpi header
#include <RInside.h> // for the embedded R via RInside

int main(int argc, char *argv[]) {

    MPI::Init(argc, argv);  // mpi initialization
    int myrank = MPI::COMM_WORLD.Get_rank();  // obtain current node rank
    int nodesize = MPI::COMM_WORLD.Get_size(); // obtain total nodes running.

    RInside R(argc, argv);  // create an embedded R instance

    std::stringstream txt;
    txt << "Hello from node " << myrank << " of " << nodesize << " nodes!" << std::endl;
    R.assign( txt.str(), "txt" );   // assign string to R variable 'txt'

    std::string evalstr = "cat(txt)";
    R.parseEvalQ( evalstr );  // eval the string, ign. any returns

    MPI::Finalize();  // mpi finalization

    exit(0);
}
```
RInside workflow

- C++ programs compute, gather or aggregate raw data.
- Data is saved and analysed before a new ’run’ is launched.
- With RInside we now skip a step:
  - collect data in a vector or matrix
  - pass data to R — easy thanks to Rcpp wrappers
  - pass one or more short ’scripts’ as strings to R to evaluate
  - pass data back to C++ programm — easy thanks to Rcpp converters
  - resume main execution based on new results

- A number of simple examples ship with RInside
Users of Rcpp

- RInside uses Rcpp for object transfer and more
- RcppArmadillo (which contains fastLM())
- RcppExamples is a ‘this is how you can do it’ stanza
- RProtoBuf is what got Romain and me here, it may get rewritten to take more advantage of Rcpp
- RQuantLib is where Rcpp originally started
- highlight is Romain’s first re-use of Rcpp
- mvabund, sdcTable, bifactorial, minqa are truly external users which are all on CRAN
- upcoming: pcaMethods (BioC), phylobase, possibly lme4
- Your package here next?
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Wrapping up

This presentation has tried to convince you that

- While the deck way be stacked against you (when adding C/C++ to R), you can still pick where to play
- R can be extended in many ways; we focus on something that allows us write extensions
  - that are efficient: we want speed and features
  - that correspond to the R object model
  - that also allow us to embed R inside C++
- And all this while retaining ’high-level’ STL-alike semantics, templates and other goodies in C++
- Using C++ abstractions wisely can keep the code both clean and readable – yet very efficient
Some pointers

- [http://cran.r-project.org/package=Rcpp](http://cran.r-project.org/package=Rcpp)
- [http://r-forge.r-project.org/projects/rcpp/](http://r-forge.r-project.org/projects/rcpp/)
- and likewise for RInside, RProtoBuf and more.
Thank you!