RcppGSL: Easier GSL use from R via Rcpp

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Abstract

The GNU Scientific Library, or **GSL**, is a collection of numerical routines for scientific computing (Galassi et al., 2010). It is particularly useful for C and C++ programs as it provides a standard C interface to a wide range of mathematical routines such as special functions, permutations, combinations, fast fourier transforms, eigensystems, random numbers, quadrature, random distributions, quasi-random sequences, Monte Carlo integration, N-tuples, differential equations, simulated annealing, numerical differentiation, interpolation, series acceleration, Chebyshev approximations, root-finding, discrete Hankel transforms physical constants, basis splines and wavelets. There are over 1000 functions in total with an extensive test suite.

The **RcppGSL** package provides an easy-to-use interface between **GSL** data structures and R using concepts from **Rcpp** (Eddelbuettel and François, 2011; Eddelbuettel, François, Allaire, Chambers, Bates, and Ushey, 2015; Eddelbuettel, 2013) which is itself a package that eases the interfaces between R and C++.

1 Introduction

The GNU Scientific Library, or **GSL**, is a collection of numerical routines for scientific computing (Galassi et al., 2010). It is a rigourously developed and tested library providing support for a wide range of scientific or numerical tasks. Among the topics covered in the GSL are complex numbers, roots of polynomials, special functions, vector and matrix data structures, permutations, combinations, sorting, BLAS support, linear algebra, fast fourier transforms, eigensystems, random numbers, quadrature, random distributions, quasi-random sequences, Monte Carlo integration, N-tuples, differential equations, simulated annealing, numerical differentiation, interpolation, series acceleration, Chebyshev approximations, root-finding, discrete Hankel transforms least-squares fitting, minimization, physical constants, basis splines and wavelets.

Support for C programming with the GSL is readily available: the GSL itself is written in C and provides a C-language Application Programming Interface (API). Access from C++ is therefore possible, albeit not at the abstraction level that can be offered by dedicated C++ implementations.¹

The GSL is somewhat unique among numerical libraries. Its combination of broad coverage of scientific topics, serious implementation effort and the use of a FLOSS license have lead to a fairly wide usage of the library. As a concrete example, we can consider the the CRAN repository network for the R language and environment (R Development Core Team, 2013). CRAN contains over a dozen packages interfacing the GSL: **copula**, **dynamo**, **gsl**, **gstat**, **magnets**, **mvabund**, **QRMlib**, **RBrownie**, **RDieHarder**, **RHmm**, **segclust**, **surveillance**, and **topicmodels**. This is a clear indication that the GSL is popular among programmers using either the C or C++ language for solving problems applied science.

At the same time, the **Rcpp** package (Eddelbuettel and François, 2011; Eddelbuettel et al., 2015) offers a higher-level abstraction between R and underlying C++ (or C) code. **Rcpp** permits R objects like vectors, matrices, lists, functions, environments, ..., to be manipulated directly at the C++ level,

¹Several C++ wrappers for the GSL have been written over the years yet none reached a state of completion comparable to the GSL itself. Three such wrapping library are http://cholm.home.cern.ch/cholm/misc/gslmm/, http://gslwrap.sourceforge.net/ and http://code.google.com/p/gslcpp/.

alleviates the needs for complicated and error-prone parameter passing and memory allocation. It also permits compact vectorised expressions similar to what can be written in R directly at the C++ level.

The **RcppGSL** package discussed here aims the help close the gap. It tries to offer access to GSL functions, in particular via the vector and matrix data structures used throughout the GSL, while staying closer to the 'whole object model' familiar to the R programmer.

The rest of paper is organised as follows. The next section shows a motivating example of a fast linear model fit routine using **GSL** functions. The following section discusses support for **GSL** vector types, which is followed by a section on matrices.

2 Motivation: FastLm

Fitting linear models is a key building block of analysing data and modeling. R has a very complete and feature-rich function in lm() which can provide a model fit as we a number of diagnostic measure, either directly or via the corresponding summary() method for linear model fits. The lm.fit() function also provides a faster alternative (which is however recommend only for for advanced users) which provides estimates only and fewer statistics for inference. This sometimes leads users request a routine which is both fast and featureful enough. The fastLm routine shown here provides such an implementation. It uses the GSL for the least-squares fitting functions and therefore provides a nice example for GSL integration with R.

```
#include <RcppGSL.h>
#include <gsl/gsl_multifit.h>
#include <cmath>
extern "C" SEXP fastLm(SEXP ys, SEXP Xs) {
  try {
        RcppGSL::vector<double> y = ys;
                                                // create gsl data structures from SEXP
        RcppGSL::matrix<double> X = Xs;
        int n = X.nrow(), k = X.ncol();
        double chisq;
        RcppGSL::vector<double> coef(k);
                                                // to hold the coefficient vector
        RcppGSL::matrix<double> cov(k,k);
                                                // and the covariance matrix
        // the actual fit requires working memory we allocate and free
        gsl_multifit_linear_workspace *work = gsl_multifit_linear_alloc (n, k);
        gsl_multifit_linear (X, y, coef, cov, &chisq, work);
        gsl_multifit_linear_free (work);
        // extract the diagonal as a vector view
        gsl_vector_view diag = gsl_matrix_diagonal(cov) ;
        // currently there is not a more direct interface in Rcpp::NumericVector
         // that takes advantage of wrap, so we have to do it in two steps
        Rcpp::NumericVector std_err ; std_err = diag;
        std::transform( std_err.begin(), std_err.end(), std_err.begin(), sqrt);
        Rcpp::List res = Rcpp::List::create(Rcpp::Named("coefficients") = coef,
                                                Rcpp::Named("stderr") = std_err,
                                                Rcpp::Named("df") = n - k);
        // free all the GSL vectors and matrices -- as these are really C data structures
        // we cannot take advantage of automatic memory management
        coef.free(); cov.free(); y.free(); X.free();
        return res;
                       // return the result list to R
  } catch( std::exception &ex ) {
        forward_exception_to_r( ex );
  } catch(...) {
         ::Rf_error( "c++ exception (unknown reason)" );
  }
  return R_NilValue; //-Wall
```

We first initialize a *RcppGSL* vector and matrix, each templated to the standard numeric type double (and the GSL supports other types ranging from lower precision floating point to signed and unsigned integers as well as complex numbers). We the reserve another vector and matrix to hold the resulting coefficient estimates as well as the estimate of the covariance matrix. Next, we allocate workspace using a GSL routine, fit the linear model and free the workspace. The next step involves extracting the diagonal element from the covariance matrix. We then employ a so-called iterator—a common C++ idiom from the Standard Template Library (STL)—to iterate over the vector of diagonal and transforming it by applying the square root function to compute our standard error of the estimate. Finally we create a named list

with the return value before we free temporary memory allocation (a step that has to be done because the underlying objects are really C objects conforming to the **GSL** interface and hence without the automatic memory management we could have with C++ vector or matrix structures as used through the **Rcpp** package) and return the result to R.

We should note that **RcppArmadillo** (François, Eddelbuettel, and Bates, 2014; Eddelbuettel and Sanderson, 2014) implements a matching fastLm function using the Armadillo library by Sanderson (2010), and can do so with more compact code due to C++ features.

3 Vectors

This section details the different vector representaions, starting with their definition inside the **GSL**. We then discuss our layering before showing how the two types map. A discussion of read-only 'vector view' classes concludes the section.

3.1 GSL Vectors

GSL defines various vector types to manipulate one-dimensionnal data, similar to R arrays. For example the gsl_vector_int structs are defined as:

```
typedef struct{
    size_t size;
    size_t stride;
    double * data;
    gsl_block * block;
    int owner;
} gsl_vector;

typedef struct {
    size_t size;
    size_t stride;
    int * data;
    gsl_block_int * block;
    int owner;
}
gsl_vector_int;
```

A typical use of the gsl_vector struct is given below:

3.2 RcppGSL::vector

RcppGSL defines the template RcppGSL::vector<T> to manipulate gsl_vector pointers taking advantage of C++ templates. Using this template type, the previous example now becomes:

The class RcppGSL::vector<double> is a smart pointer, that can be used anywhere where a raw pointer gsl_vector can be used, such as the gsl_vector_set and gsl_vector_get functions above.

Beyond the convenience of a nicer syntax for allocation and release of memory, the RcppGSL::vector template faciliates interchange of **GSL** vectors with **Rcpp** objects, and hence **R** objects. The following example defines a .Call compatible function called sum_gsl_vector_int that operates on a gsl_vector_int through the RcppGSL::vector<int> template specialization:

```
//[[Rcpp::export]]
int sum_gsl_vector_int( RcppGSL::vector<int> vec){
  int res = std::accumulate( vec.begin(), vec.end(), 0 );
  vec.free(); // we need to free vec after use
  return res;
}
```

p The function can then simply be called from R:

```
> .Call( "sum_gsl_vector_int", 1:10 )
[1] 55
```

A second example shows a simple function that grabs elements of an R list as gsl_vector objects using implicit conversion mechanisms of **Rcpp**

```
//[[Rcpp::export]]
double gsl_vector_sum_2( Rcpp::List data ){
   // grab "x" as a gsl_vector through the RcppGSL::vector<double> class
   RcppGSL::vector<double> x = data["x"] ;

   // grab "y" as a gsl_vector through the RcppGSL::vector<int> class
   RcppGSL::vector<int> y = data["y"] ;
   double res = 0.0 ;
   for( size_t i=0; i < x->size; i++){
      res += x[i] * y[i] ;
   }

   // as usual with GSL, we need to explicitely free the memory
   x.free() ;
   y.free() ;

   // return the result
   return res ;
}
```

called from R:

```
> data <- list( x = seq(0,1,length=10), y = 1:10 )
> .Call( "gsl_vector_sum_2", data )
[1] 36.66667
```

3.3 Mapping

Table 1 shows the mapping between types defined by the **GSL** and their corresponding types in the **RcppGSL** package.

gsl vector	RcppGSL
gsl_vector	RcppGSL::vector <double></double>
gsl_vector_int	<pre>RcppGSL::vector<int></int></pre>
gsl_vector_float	<pre>RcppGSL::vector<float></float></pre>
gsl_vector_long	RcppGSL::vector <long></long>
gsl_vector_char	<pre>RcppGSL::vector<char></char></pre>
gsl_vector_complex	<pre>RcppGSL::vector<gsl_complex></gsl_complex></pre>
gsl_vector_complex_float	<pre>RcppGSL::vector<gsl_complex_float></gsl_complex_float></pre>
gsl_vector_complex_long_double	<pre>RcppGSL::vector<gsl_complex_long_double></gsl_complex_long_double></pre>
gsl_vector_long_double	<pre>RcppGSL::vector<long double=""></long></pre>
gsl_vector_short	RcppGSL::vector <short></short>
gsl_vector_uchar	RcppGSL::vector <unsigned char=""></unsigned>
gsl_vector_uint	RcppGSL::vector <unsigned int=""></unsigned>
gsl_vector_ushort	RcppGSL::vector <insigned short=""></insigned>
gsl_vector_ulong	<pre>RcppGSL::vector<unsigned long=""></unsigned></pre>

Table 1: Correspondance between GSL vector types and templates defined in RcppGSL.

3.4 Vector Views

Several **GSL** algorithms return **GSL** vector views as their result type. **RcppGSL** defines the template class RcppGSL::vector_view to handle vector views using C++ syntax.

As with vectors, C++ objects of type RcppGSL::vector_view can be converted implicitly to their associated **GSL** view type. Table 2 displays the pairwise correspondance so that the C++ objects can be passed to compatible **GSL** algorithms.

gsl vector views	RcppGSL
gsl_vector_view	RcppGSL::vector_view <double></double>
gsl_vector_view_int	<pre>RcppGSL::vector_view<int></int></pre>
gsl_vector_view_float	<pre>RcppGSL::vector_view<float></float></pre>
gsl_vector_view_long	<pre>RcppGSL::vector_view<long></long></pre>
gsl_vector_view_char	<pre>RcppGSL::vector_view<char></char></pre>
gsl_vector_view_complex	<pre>RcppGSL::vector_view<gsl_complex></gsl_complex></pre>
gsl_vector_view_complex_float	<pre>RcppGSL::vector_view<gsl_complex_float></gsl_complex_float></pre>
gsl_vector_view_complex_long_double	<pre>RcppGSL::vector_view<gsl_complex_long_double></gsl_complex_long_double></pre>
gsl_vector_view_long_double	<pre>RcppGSL::vector_view<long double=""></long></pre>
gsl_vector_view_short	<pre>RcppGSL::vector_view<short></short></pre>
gsl_vector_view_uchar	<pre>RcppGSL::vector_view<unsigned char=""></unsigned></pre>
gsl_vector_view_uint	<pre>RcppGSL::vector_view<unsigned int=""></unsigned></pre>
gsl_vector_view_ushort	<pre>RcppGSL::vector_view<insigned short=""></insigned></pre>
gsl_vector_view_ulong	<pre>RcppGSL::vector_view<unsigned long=""></unsigned></pre>

Table 2: Correspondance between GSL vector view types and templates defined in RcppGSL.

The vector view class also contains a conversion operator to automatically transform the data of the view object to a **GSL** vector object. This enables use of vector views where **GSL** would expect a vector.

4 Matrices

The **GSL** also defines a set of matrix data types: gsl_matrix, gsl_matrix_int etc ... for which **RcppGSL** defines a corresponding convenience C++ wrapper generated by the RcppGSL::matrix template.

4.1 Creating matrices

The RcppGSL::matrix template exposes three constructors.

```
// convert an R matrix to a GSL matrix
matrix( SEXP x) throw(::Rcpp::not_compatible)

// encapsulate a GSL matrix pointer
matrix( gsl_matrix* x)

// create a new matrix with the given number of rows and columns
matrix( int nrow, int ncol)
```

4.2 Implicit conversion

RcppGSL::matrix defines implicit conversion to a pointer to the associated **GSL** matrix type, as well as dereferencing operators, making the class RcppGSL::matrix look and feel like a pointer to a GSL matrix type.

```
gsltype* data ;
operator gsltype*(){ return data ; }
gsltype* operator->() const { return data; }
gsltype& operator*() const { return *data; }
```

4.3 Indexing

Indexing of **GSL** matrices is usually the task of the functions gsl_matrix_get, gsl_matrix_int_get, ... and gsl_matrix_set, gsl_matrix_int_set, ...

RcppGSL takes advantage of both operator overloading and templates to make indexing a **GSL** matrix much more convenient.

4.4 Methods

The RcppGSL::matrix type also defines the following member functions:

```
nrow extracts the number of rows
ncol extract the number of columns
size extracts the number of elements
free releases the memory
```

4.5 Matrix views

Similar to the vector views discussed above, the **RcppGSL** also provides an implicit conversion operator which returns the underlying matrix stored in the matrix view class.

5 Error handler

When input values for **GSL** functions are invalid, the default error handler will abort the program after printing an error message, which will lead R to an abortion error. To avoid this, we need to close it first by using gsl_set_error_handler_off() and then detect the result is NAN or not.

```
// close the GSL error handler
gsl_set_error_handler_off();

// feed GSL function with some invalid values
double res = gsl_sf_hyperg_2F1(1, 1, 1.1467003, 1);

// detect the result is NAN or not
if (ISNAN(res)){
    Rcpp::Rcout << "Invalid input found!" << std::endl;
}</pre>
```

See http://thread.gmane.org/gmane.comp.lang.r.rcpp/7905 for a longer discussion.

Starting with release 0.2.4, two new functions are available: gslSetErrorHandlerOff() and gslResetErrorHandler() which can allow to turn off the error handler (as discussed above), and to reset to the prior (default) value.

In addition, the package now also calls gslSetErrorHandlerOff() when being attached, ensuring that the GSL error handler is turned off by default.

6 Using RcppGSL in your package

The **RcppGSL** package contains a complete example providing a single function colNorm which computes a norm for each column of a supplied matrix. This example adapts a matrix example from the GSL manual that has been chose merely as a means to showing how to set up a package to use **RcppGSL**.

Needless to say, we could compute such a matrix norm easily in R using existing facilities. One such possibility is a simple apply(M, 2, function(x) sqrt(sum(x^2))) as shown on the corresponding help page in the example package inside RcppGSL. One point in favour of using the GSL code is that it employs a BLAS function so on sufficiently large matrices, and with suitable BLAS libraries installed, this variant could be faster due to the optimised code in high-performance BLAS libraries and/or the inherent parallelism a multi-core BLAS variant which compute compute the vector norm in parallel. On all 'reasonable' matrix sizes, however, the performance difference should be neglible.

6.1 The configure script

6.1.1 Using autoconf

Using **RcppGSL** means employing both the **GSL** and R. We may need to find the location of the **GSL** headers and library, and this done easily from a configure source script which autoconf generates from a configure.in source file such as the following:

```
AC_INIT([RcppGSLExample], 0.1.0)
## Use gsl-config to find arguments for compiler and linker flags
## Check for non-standard programs: gsl-config(1)
AC_PATH_PROG([GSL_CONFIG], [gsl-config])
## If gsl-config was found, let's use it
if test "${GSL_CONFIG}" != ""; then
    # Use gsl-config for header and linker arguments (without BLAS which we get from R)
    GSL_CFLAGS='${GSL_CONFIG} --cflags'
    GSL_LIBS='${GSL_CONFIG} --libs-without-cblas'
else
    AC_MSG_ERROR([gsl-config not found, is GSL installed?])
fi
# Now substitute these variables in src/Makevars.in to create src/Makevars
AC_SUBST(GSL_CFLAGS)
AC_SUBST(GSL_LIBS)
AC_OUTPUT(src/Makevars)
```

Such a source configure.in gets converted into a script configure by invoking the autoconf program.

6.1.2 Using functions provided by RcppGSL

RcppGSL provides R functions that allows one to retrieve the same information. Therefore the configure script can also be written as:

```
#!/bin/sh

GSL_CFLAGS='${R_HOME}/bin/Rscript -e "RcppGSL:::CFlags()"'
GSL_LIBS='${R_HOME}/bin/Rscript -e "RcppGSL:::LdFlags()"'

sed -e "s|@GSL_LIBS@|${GSL_LIBS}|" \
    -e "s|@GSL_CFLAGS@|${GSL_CFLAGS}|" \
    src/Makevars.in > src/Makevars
```

Similarly, the configure.win for windows can be written as:

```
GSL_CFLAGS='${R_HOME}/bin${R_ARCH_BIN}/Rscript.exe -e "RcppGSL:::CFlags()"'
GSL_LIBS='${R_HOME}/bin${R_ARCH_BIN}/Rscript.exe -e "RcppGSL:::LdFlags()"'
sed -e "s|@GSL_LIBS@|${GSL_LIBS}|" \
    -e "s|@GSL_CFLAGS@|${GSL_CFLAGS}|" \
    src/Makevars.in > src/Makevars.win
```

6.2 The src directory

The C++ source file takes the matrix supplied from R and applies the **GSL** function to each column.

```
#include <RcppGSL.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>
extern "C" SEXP colNorm(SEXP sM) {
  try {
        RcppGSL::matrix<double> M = sM;  // create gsl data structures from SEXP
        int k = M.ncol();
        Rcpp::NumericVector n(k);
                                              // to store results
        for (int j = 0; j < k; j++) {
            RcppGSL::vector_view<double> colview = gsl_matrix_column (M, j);
            n[j] = gsl_blas_dnrm2(colview);
        M.free();
                                             // return vector
        return n;
 } catch( std::exception &ex ) {
        forward_exception_to_r( ex );
  } catch(...) {
        ::Rf_error( "c++ exception (unknown reason)" );
 }
  return R_NilValue; //-Wall
```

The Makevars.in file governs the compilation and uses the values supplied by configure during build-time:

```
# set by configure

GSL_CFLAGS = @GSL_CFLAGS@

GSL_LIBS = @GSL_LIBS@

# combine with standard arguments for R

PKG_CPPFLAGS = $(GSL_CFLAGS)

PKG_LIBS = $(GSL_LIBS)
```

The variables surrounded by will be filled by configure during package build-time.

6.3 The R directory

The R source is very simply: a single matrix is passed to C++:

```
> colNorm <- function(M) {
+    stopifnot(is.matrix(M))
+    res <- .Call("colNorm", M, package="RcppGSLExample")
+ }</pre>
```

7 Using RcppGSL with inline

The **inline** package (Sklyar, Murdoch, Smith, Eddelbuettel, and François, 2013) is very helpful for prototyping code in C, C++ or Fortran as it takes care of code compilation, linking and dynamic loading directly from R. It is being used extensively by **Rcpp**, for example in the numerous unit tests.

The example below shows how **inline** can be deployed with **RcppGSL**. We implement the same column norm example, but this time as an R script which is compiled, linked and loaded on-the-fly. Compared to standard use of **inline**, we have to make sure to add a short section declaring which header files from **GSL** we need to use; the **RcppGSL** then communicates with **inline** to tell it about the location and names of libraries used to build code against **GSL**.

```
> require(inline)
> inctxt='
   #include <gsl/gsl_matrix.h>
   #include <gsl/gsl_blas.h>
> bodytxt='
  RcppGSL::matrix<double> M = sM; // create gsl data structures from
  int k = M.ncol();
                                     // to store results
  Rcpp::NumericVector n(k);
 for (int j = 0; j < k; j++) {
   RcppGSL::vector_view<double> colview = gsl_matrix_column (M, j);
   n[j] = gsl_blas_dnrm2(colview);
  M.free();
                                      // return vector
  return n;
> foo <- cxxfunction(</pre>
      signature(sM="numeric"),
      body=bodytxt, inc=inctxt, plugin="RcppGSL")
> M \leftarrow outer(sin(0:9), rep(1,10), "*") + outer(rep(1, 10), cos(0:9), "*")
> foo(M)
 [1] 4.314614 3.120504 2.193159 3.261141 2.534157 2.572810
 [7] 4.204689 3.652017 2.085236 3.073134
```

The RcppGSL inline plugin supports creation of a package skeleton based on the inline function.

```
> package.skeleton( "mypackage", foo )
```

8 Using RcppGSL with Rcpp Attributes

Rcpp Attributes (Allaire, Eddelbuettel, and François, 2013) builds on the features of the **inline** package described in previous section, and streamline the compilation, loading and linking process even further. It leverages the existing plugins for **inline**. This section illustrates how the example from the previous section can be written using *Rcpp Attributes*.

```
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>
#include <RcppGSL.h>
// declare a dependency on the RcppGSL package; also activates plugin
// [[Rcpp::depends(RcppGSL)]]
// declare the function to be 'exported' to R
// [[Rcpp::export]]
Rcpp::NumericVector foo(Rcpp::NumericMatrix sM) {
    RcppGSL::matrix<double> M = Rcpp::as<RcppGSL::matrix<double> >(sM);
    int k = M.ncol();
    Rcpp::NumericVector n(k);
                                            // to store results
    for (int j = 0; j < k; j++) {
 RcppGSL::vector_view<double> colview = gsl_matrix_column (M, j);
 n[j] = gsl_blas_dnrm2(colview);
    M.free();
                                            // return vector
    return n;
}
/*** R
## see Section 8.4.13 of the GSL manual:
## create M as a sum of two outer products
M \leftarrow outer(sin(0:9), rep(1,10), "*") +
     outer(rep(1, 10), cos(0:9), "*")
foo(M)
```

With the code above stored in a file, say, "gslNorm.cpp" one can simply call sourceCpp() to have the wrapper code added, and all of the compilation, linking and loading done — including the execution of the short R segment at the end:

```
> sourceCpp("gslNorm.cpp")
```

See the vignette "Rcpp-attributes" (Allaire et al., 2013) of the **Rcpp** package (Eddelbuettel et al., 2015) for details.

9 Summary

The GNU Scientific Library (GSL) by Galassi et al. (2010) offers a very comprehensive collection of rigorously developed and tested functions for applied scientific computing under a common Open Source license. This has lead to widespread deployment of **GSL** among a number of disciplines.

Using the automatic wrapping and converters offered by the **RcppGSL** package presented here, R users and programmers can now deploy algorithms provided by the **GSL** with greater ease.

References

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