An Introduction to **RcppEigen**

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RcppEigen version 0.1.4 as of November 1, 2011

Abstract

The **RcppEigen** package provides access from R (R Development Core Team, 2011b) to the **Eigen** C++ template library for numerical linear algebra. **Rcpp** (Eddelbuettel and François, 2011b) classes and specializations of the C++ templated functions `as` and `wrap` from **Rcpp** provide the "glue" for passing objects from R to C++ and back.

1 Introduction

Linear algebra is an essential building block of statistical computing. Operations such as matrix decompositions, linear program solvers, and eigenvalue / eigenvector computations are used in many estimation and analysis routines. As such, libraries supporting linear algebra have long been provided by statistical programmers for different programming languages and environments. C++, one of the central modern languages for numerical and statistical computing, can be extended particularly well due to its object-oriented nature, and numerous class libraries providing linear algebra routines have been written over the years.

As both the C++ language and standards have evolved (Meyers, 2005, 1995), so have the compilers implementing the language. Relatively modern language constructs such as template meta-programming are particularly useful. It provides both overloading of operations (allowing expressive code in the compiled language similar to what can be done in scripting languages) and can shift some of the computational burden from the run-time to the compile-time (though a more detailed discussions of template programming is however beyond this paper). Veldhuizen (1998) provided an early and influential implementation that already demonstrated key features of this approach. Its usage however was held back at the time by the somewhat limited availability of compilers implementing all necessary features of the C++ language.

This situation has greatly improved over the last decade, and many more such libraries have been contributed. One such C++ library is **Eigen** by Guennebaud, Jacob, et al. (2011). **Eigen** started as a sub-project to KDE (a popular Linux desktop environment), initially focussing on fixed-size matrices which are projections in a visualization application. **Eigen** grew from there and has over the course of about a decade produced three major releases with "Eigen3" being the current version.

Eigen is of interest as the R system for statistical computation and graphics (R Development Core Team, 2011b) is itself easily extensible. This is particular true via the C language that most of R's compiled core parts are written in, but also for the C++ language which can interface with C-based systems rather easily. The manual "Writing R Extensions" (R Development Core Team, 2011a) is the basic reference for extending R with either C or C++.

The **Rcpp** package by Eddelbuettel and François (2011a) facilitates extending R with C++ code by providing seamless object mapping between both languages. As stated in the **Rcpp** (Eddelbuettel and François, 2011a) vignette, "Extending **Rcpp**"

> **Rcpp** facilitates data interchange between R and C++ through the templated functions `Rcpp::as` (for conversion of objects from R to C++) and `Rcpp::wrap` (for conversion from C++ to R).

The **RcppEigen** package provides the header files composing the **Eigen** C++ template library and implementations of `Rcpp::as` and `Rcpp::wrap` for the C++ classes defined in **Eigen**.

The **Eigen** classes themselves provide high-performance, versatile and comprehensive representations of dense and sparse matrices and vectors, as well as decompositions and other functions to be applied to these objects. The next section introduces some of these classes and shows how to interface to them from R.

2 Eigen classes

Eigen (Guennebaud, Jacob, et al., 2011) is a C++ template library providing classes for many forms of matrices, vectors, arrays and decompositions. These classes are flexible and comprehensive allowing for both high performance and well structured code representing high-level operations. C++ code based on Eigen is often more like R code, working on the "whole object", rather than compiled code in other languages where operations often must be coded in loops.

As in many C++ template libraries using template meta-programming (Abrahams and Gurtovoy, 2004), the templates themselves can be very complicated. However, **Eigen** provides `typedef`s for common classes that correspond to R matrices and vectors, as shown in Table 1, and this paper will use these `typedef`s throughout this document.

The C++ classes shown in Table 1 are in the `Eigen` namespace, which means that they must be written as `Eigen::MatrixXd`. However, if one prefaces the use of these class names with a declaration like

```
using Eigen::MatrixXd;
```

then one can use these names without the namespace qualifier.

2.1 Mapped matrices in Eigen

Storage for the contents of matrices from the classes shown in Table 1 is allocated and controlled by the class constructors and destructors. Creating an instance of such a class from an R object involves copying its contents. An alternative is to have the contents of the R matrix or vector mapped to the contents of the object from the Eigen class. For dense matrices one can use the Eigen templated class `Map`, and for sparse matrices one can deploy the Eigen templated class `MappedSparseMatrix`.

One must, of course, be careful not to modify the contents of the R object in the C++ code. A recommended practice is always to declare mapped objects as `const`.

2.2 Arrays in Eigen

For matrix and vector classes **Eigen** overloads the `'*'` operator to indicate matrix multiplication. Occasionally component-wise operations instead of matrix operations are preferred. The `Array` templated classes are used in **Eigen** for component-wise operations. Most often the `array()` method is used for Matrix or Vector objects to create the array. On those occasions when one wishes to convert an array to a matrix or vector object the `matrix()` method is used.

2.3 Structured matrices in Eigen

There are **Eigen** classes for matrices with special structure such as symmetric matrices, triangular matrices and banded matrices. For dense matrices, these special structures are described as "views", meaning that the full dense matrix is stored but only part of the matrix is used in operations. For a symmetric matrix one needs to specify whether the lower triangle or the upper triangle is to be used as the contents, with the other triangle defined by the implicit symmetry.

Table 1: Correspondence between R matrix and vector types and classes in the `Eigen` namespace.

R object type	**Eigen** class typedef
numeric matrix	`MatrixXd`
integer matrix	`MatrixXi`
complex matrix	`MatrixXcd`
numeric vector	`VectorXd`
integer vector	`VectorXi`
complex vector	`VectorXcd`
`Matrix::dgCMatrix`	`SparseMatrix<double>`

3 Some simple examples

C++ functions to perform simple operations on matrices or vectors can follow a pattern of:

1. Map the R objects passed as arguments into Eigen objects.
2. Create the result.
3. Return `Rcpp::wrap` applied to the result.

An idiom for the first step is

```
using Eigen::Map;
using Eigen::MatrixXd;
using Rcpp::as;

const Map<MatrixXd>  A(as<Map<MatrixXd> >(AA));
```

where `AA` is the name of the R object (called an `SEXP` in C and C++) passed to the C++ function.

The `cxxfunction` from the **inline** package (Sklyar, Murdoch, Smith, Eddelbuettel, and François, 2010) for R and its **RcppEigen** plugin provide a convenient way of developing and debugging the C++ code. For actual production code one generally incorporates the C++ source code files in a package and include the line `LinkingTo: Rcpp, RcppEigen` in the package's `DESCRIPTION` file. The `RcppEigen.package.skeleton` function provides a quick way of generating the skeleton of a package using **RcppEigen** facilities.

The `cxxfunction` with the `"Rcpp"` or `"RcppEigen"` plugins has the `as` and `wrap` functions already defined as `Rcpp::as` and `Rcpp::wrap`. In the examples below these declarations are omitted. It is important to remember that they are needed in actual C++ source code for a package.

The first few examples are simply for illustration as the operations shown could be more effectively performed directly in R. Finally, the results from **Eigen** are compared to those from the direct R results.

3.1 Transpose of an integer matrix

The next R code snippet creates a simple matrix of integers

```
> (A <- matrix(1:6, ncol=2))
```

```
     [,1] [,2]
[1,]    1    4
[2,]    2    5
[3,]    3    6
```

```
> str(A)
```

```
 int [1:3, 1:2] 1 2 3 4 5 6
```

and, in Figure 1, the `transpose()` method for the `Eigen::MatrixXi` class is used to return the transpose of the supplied matrix. The R matrix in the `SEXP AA` is mapped to an `Eigen::MatrixXi` object then the matrix `At` is constructed from its transpose and returned to R.

```
using Eigen::Map;
using Eigen::MatrixXi;
                    // Map the integer matrix AA from R
const Map<MatrixXi>  A(as<Map<MatrixXi> >(AA));
                    // evaluate and return the transpose of A
const MatrixXi       At(A.transpose());
return wrap(At);
```

Figure 1: **transCpp**: Transpose a matrix of integers

The next R snippet compiles and links the C++ code segment (stored as text in a variable named `transCpp`) into an executable function `ftrans` and then checks that it works as intended by compariing the output to an explicit transpose of the matrix argument.

```
> ftrans <- cxxfunction(signature(AA="matrix"), transCpp, plugin="RcppEigen")
> (At <- ftrans(A))
```

```
     [,1] [,2] [,3]
[1,]    1    2    3
[2,]    4    5    6
```

```
> stopifnot(all.equal(At, t(A)))
```

For numeric or integer matrices the `adjoint()` method is equivalent to the `transpose()` method. For complex matrices, the adjoint is the conjugate of the transpose. In keeping with the conventions in the **Eigen** documentation, in what follows, the `adjoint()` method is used to create the transpose of numeric or integer matrices.

3.2 Products and cross-products

As mentioned in Sec. 2.2, the '`*`' operator performs matrix multiplication on `Eigen::Matrix` or `Eigen::Vector` objects. The C++ code in Figure 2 produces a list containing both the product and cross-product of its two arguments.

```
using Eigen::Map;
using Eigen::MatrixXi;
const Map<MatrixXi>    B(as<Map<MatrixXi> >(BB));
const Map<MatrixXi>    C(as<Map<MatrixXi> >(CC));
return List::create(_["B %*% C"]         = B * C,
                    _["crossprod(B, C)"] = B.adjoint() * C);
```

Figure 2: **prodCpp**: Product and cross-product of two matrices

```
> fprod <- cxxfunction(signature(BB = "matrix", CC = "matrix"), prodCpp, "RcppEigen")
> B <- matrix(1:4, ncol=2); C <- matrix(6:1, nrow=2)
> str(fp <- fprod(B, C))
```

```
List of 2
 $ B %*% C        : int [1:2, 1:3] 21 32 13 20 5 8
 $ crossprod(B, C): int [1:2, 1:3] 16 38 10 24 4 10
```

```
> stopifnot(all.equal(fp[[1]], B %*% C), all.equal(fp[[2]], crossprod(B, C)))
```

Notice that the `create` method for the **Rcpp** class `List` implicitly applies `Rcpp::wrap` to its arguments.

3.3 Crossproduct of a single matrix

As shown in the last example, the R function `crossprod` calculates the product of the transpose of its first argument with its second argument. The single argument form, `crossprod(X)`, evaluates $\boldsymbol{X}'\boldsymbol{X}$. One could, of course, calculate this product as

```
> t(X) %*% X
```

but `crossprod(X)` is roughly twice as fast because the result is known to be symmetric and only one triangle needs to be calculated. The function `tcrossprod` evaluates `crossprod(t(X))` without actually forming the transpose.

To express these calculations in Eigen, a `SelfAdjointView` is created, which is a dense matrix of which only one triangle is used, the other triangle being inferred from the symmetry. ("Self-adjoint" is equivalent to symmetric for non-complex matrices.)

The **Eigen** class name is `SelfAdjointView`. The method for general matrices that produces such a view is called `selfadjointView`. Both require specification of either the `Lower` or `Upper` triangle.

For triangular matrices the class is `TriangularView` and the method is `triangularView`. The triangle can be specified as `Lower`, `UnitLower`, `StrictlyLower`, `Upper`, `UnitUpper` or `StrictlyUpper`.

For self-adjoint views the `rankUpdate` method adds a scalar multiple of $\boldsymbol{A}\boldsymbol{A}'$ to the current symmetric matrix. The scalar multiple defaults to 1. The code in Figure 3 produces

```
using Eigen::Map;
using Eigen::MatrixXi;
using Eigen::Lower;

const Map<MatrixXi> A(as<Map<MatrixXi> >(AA));
const int           m(A.rows()), n(A.cols());
MatrixXi          AtA(MatrixXi(n, n).setZero().
                      selfadjointView<Lower>().rankUpdate(A.adjoint()));
MatrixXi          AAt(MatrixXi(m, m).setZero().
                      selfadjointView<Lower>().rankUpdate(A));

return List::create(_["crossprod(A)"]  = AtA,
                    _["tcrossprod(A)"] = AAt);
```

Figure 3: **crossprodCpp**: Cross-product and transposed cross-product of a single matrix

```
> fcprd <- cxxfunction(signature(AA = "matrix"), crossprodCpp, "RcppEigen")
> str(crp <- fcprd(A))

List of 2
 $ crossprod(A) : int [1:2, 1:2] 14 32 32 77
 $ tcrossprod(A): int [1:3, 1:3] 17 22 27 22 29 36 27 36 45

> stopifnot(all.equal(crp[[1]], crossprod(A)), all.equal(crp[[2]], tcrossprod(A)))
```

To some, the expressions to construct `AtA` and `AAt` in that code fragment are compact and elegant. To others they are hopelessly confusing. If you find yourself in the latter group, you just need to read the expression left to right. So, for example, we construct `AAt` by creating a general integer matrix of size $m \times m$ (where $\boldsymbol{A}$ is $m \times n$), ensure that all its elements are zero, regard it as a self-adjoint (i.e. symmetric) matrix using the elements in the lower triangle, then add $\boldsymbol{AA}'$ to it and convert back to a general matrix form (i.e. the strict lower triangle is copied into the strict upper triangle).

For these products one could use either the lower triangle or the upper triangle as the result will be symmetrized before it is returned.

3.4 Cholesky decomposition of the crossprod

The Cholesky decomposition of the positive-definite, symmetric matrix, $\boldsymbol{A}$, can be written in several forms. Numerical analysts define the "LLt" form as the lower triangular matrix, $\boldsymbol{L}$, such that $\boldsymbol{A} = \boldsymbol{LL}'$ and the "LDLt" form as a unit lower triangular matrix $\boldsymbol{L}$ and a diagonal matrix $\boldsymbol{D}$ with positive diagonal elements such that $\boldsymbol{A} = \boldsymbol{LDL}'$. Statisticians often write the decomposition as $\boldsymbol{A} = \boldsymbol{R}'\boldsymbol{R}$ where $\boldsymbol{R}$ is an upper triangular matrix. Of course, this $\boldsymbol{R}$ is simply the transpose of $\boldsymbol{L}$ from the "LLt" form.

The templated **Eigen** classes for the LLt and LDLt forms are called `LLT` and `LDLT`. In general, one would preserve the objects from these classes in order to re-use them for solutions of linear systems. For a simple illustration, the matrix $\boldsymbol{L}$ from the "LLt" form is returned.

Because the Cholesky decomposition involves taking square roots, the internal representation is switched to numeric matrices

```
> storage.mode(A) <- "double"
```

before applying the code in Figure 4.

```
> fchol <- cxxfunction(signature(AA = "matrix"), cholCpp, "RcppEigen")
> (ll <- fchol(A))

$L
         [,1]     [,2]
[1,] 3.741657 0.000000
[2,] 8.552360 1.963961

$R
         [,1]     [,2]
```

```
using Eigen::Map;
using Eigen::MatrixXd;
using Eigen::LLT;
using Eigen::Lower;

const Map<MatrixXd>   A(as<Map<MatrixXd> >(AA));
const int             n(A.cols());
const LLT<MatrixXd> llt(MatrixXd(n, n).setZero().
                        selfadjointView<Lower>().rankUpdate(A.adjoint()));

return List::create(_["L"] = MatrixXd(llt.matrixL()),
                    _["R"] = MatrixXd(llt.matrixU()));
```

Figure 4: **cholCpp**: Cholesky decomposition of a cross-product

```
[1,] 3.741657 8.552360
[2,] 0.000000 1.963961
```

```
> stopifnot(all.equal(ll[[2]], chol(crossprod(A))))
```

3.5 Determinant of the cross-product matrix

The "D-optimal" criterion for experimental design chooses the design that maximizes the determinant, $|\boldsymbol{X}'\boldsymbol{X}|$, for the $n \times p$ model matrix (or Jacobian matrix), $\boldsymbol{X}$. The determinant, $|\boldsymbol{L}|$, of the $p \times p$ lower Cholesky factor $\boldsymbol{L}$, defined so that $\boldsymbol{L}\boldsymbol{L}' = \boldsymbol{X}'\boldsymbol{X}$, is the product of its diagonal elements, as is the case for any triangular matrix. By the properties of determinants,

$$|\boldsymbol{X}'\boldsymbol{X}| = |\boldsymbol{L}\boldsymbol{L}'| = |\boldsymbol{L}|\,|\boldsymbol{L}'| = |\boldsymbol{L}|^2$$

Alternatively, if using the "LDLt" decomposition, $\boldsymbol{L}\boldsymbol{D}\boldsymbol{L}' = \boldsymbol{X}'\boldsymbol{X}$ where $\boldsymbol{L}$ is unit lower triangular and $\boldsymbol{D}$ is diagonal then $|\boldsymbol{X}'\boldsymbol{X}|$ is the product of the diagonal elements of $\boldsymbol{D}$. Because it is known that the diagonals of $\boldsymbol{D}$ must be non-negative, one often evaluates the logarithm of the determinant as the sum of the logarithms of the diagonal elements of $\boldsymbol{D}$. Several options are shown in Figure 5.

```
using Eigen::Lower;
using Eigen::Map;
using Eigen::MatrixXd;
using Eigen::VectorXd;

const Map<MatrixXd>   A(as<Map<MatrixXd> >(AA));
const int             n(A.cols());
const MatrixXd      AtA(MatrixXd(n, n).setZero().
                        selfadjointView<Lower>().rankUpdate(A.adjoint()));
const MatrixXd     Lmat(AtA.llt().matrixL());
const double       detL(Lmat.diagonal().prod());
const VectorXd     Dvec(AtA.ldlt().vectorD());

return List::create(_["d1"] = detL * detL,
                    _["d2"] = Dvec.prod(),
                    _["ld"] = Dvec.array().log().sum());
```

Figure 5: **cholDetCpp**: Determinant of a cross-product using the Cholesky decomposition

```
> fdet <- cxxfunction(signature(AA = "matrix"), cholDetCpp, "RcppEigen")
> unlist(ll <- fdet(A))
```

```
      d1        d2        ld
54.000000 54.000000  3.988984
```

Note the use of the `array()` method in the calculation of the log-determinant. Because the `log()` method applies to arrays, not to vectors or matrices, an array from `Dvec` has to be created before applying the `log()` method.

4 Least squares solutions

A common operation in statistical computing is calculating a least squares solution, $\widehat{\boldsymbol{\beta}}$, defined as

$$\widehat{\boldsymbol{\beta}} = \arg\min_{\beta} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|^2$$

where the model matrix, $\boldsymbol{X}$, is $n \times p$ ($n \geq p$) and $\boldsymbol{y}$ is an n-dimensional response vector. There are several ways, based on matrix decompositions, to determine such a solution. Earlier, two forms of the Cholesky decomposition were discussed: "LLt" and "LDLt", which can both be used to solve for $\widehat{\boldsymbol{\beta}}$. Other decompositions that can be used are the QR decomposition, with or without column pivoting, the singular value decomposition and the eigendecomposition of a symmetric matrix.

Determining a least squares solution is relatively straightforward. However, statistical computing often requires additional information, such as the standard errors of the coefficient estimates. Calculating these involves evaluating the diagonal elements of $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ and the residual sum of squares, $\|\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}\|^2$.

4.1 Least squares using the "LLt" Cholesky

```
using Eigen::LLT;
using Eigen::Lower;
using Eigen::Map;
using Eigen::MatrixXd;
using Eigen::VectorXd;

const Map<MatrixXd>   X(as<Map<MatrixXd> >(XX));
const Map<VectorXd>   y(as<Map<VectorXd> >(yy));
const int             n(X.rows()), p(X.cols());
const LLT<MatrixXd> llt(MatrixXd(p, p).setZero().
                        selfadjointView<Lower>().rankUpdate(X.adjoint()));
const VectorXd  betahat(llt.solve(X.adjoint() * y));
const VectorXd   fitted(X * betahat);
const VectorXd    resid(y - fitted);
const int            df(n - p);
const double          s(resid.norm() / std::sqrt(double(df)));
const VectorXd       se(s * llt.matrixL().solve(MatrixXd::Identity(p, p)).
                        colwise().norm());
return     List::create(_["coefficients"]   = betahat,
                        _["fitted.values"]  = fitted,
                        _["residuals"]      = resid,
                        _["s"]              = s,
                        _["df.residual"]    = df,
                        _["rank"]           = p,
                        _["Std. Error"]     = se);
```

Figure 6: **lltLSCpp**: Least squares using the Cholesky decomposition

Figure 6 shows a calculation of the least squares coefficient estimates (`betahat`) and the standard errors (`se`) through an "LLt" Cholesky decomposition of the crossproduct of the model matrix, $\boldsymbol{X}$. Next, the results from this calculation are compared to those from the `lm.fit` function in R (`lm.fit` is the workhorse function called by `lm` once the model matrix and response have been evaluated).

```
> lltLS <- cxxfunction(signature(XX = "matrix", yy = "numeric"), lltLSCpp, "RcppEigen")
> data(trees, package="datasets")
> str(lltFit <- with(trees, lltLS(cbind(1, log(Girth)), log(Volume))))

List of 7
 $ coefficients : num [1:2] -2.35 2.2
 $ fitted.values: num [1:31] 2.3 2.38 2.43 2.82 2.86 ...
 $ residuals    : num [1:31] 0.0298 -0.0483 -0.1087 -0.0223 0.0727 ...
 $ s            : num 0.115
 $ df.residual  : int 29
 $ rank         : int 2
 $ Std. Error   : num [1:2] 0.2307 0.0898

> str(lmFit <- with(trees, lm.fit(cbind(1, log(Girth)), log(Volume))))

List of 8
 $ coefficients : Named num [1:2] -2.35 2.2
  ..- attr(*, "names")= chr [1:2] "x1" "x2"
 $ residuals    : num [1:31] 0.0298 -0.0483 -0.1087 -0.0223 0.0727 ...
 $ effects      : Named num [1:31] -18.2218 2.8152 -0.1029 -0.0223 0.0721 ...
  ..- attr(*, "names")= chr [1:31] "x1" "x2" "" "" ...
 $ rank         : int 2
 $ fitted.values: num [1:31] 2.3 2.38 2.43 2.82 2.86 ...
 $ assign       : NULL
 $ qr           :List of 5
  ..$ qr   : num [1:31, 1:2] -5.57 0.18 0.18 0.18 0.18 ...
  ..$ qraux: num [1:2] 1.18 1.26
  ..$ pivot: int [1:2] 1 2
  ..$ tol  : num 1e-07
  ..$ rank : int 2
  ..- attr(*, "class")= chr "qr"
 $ df.residual  : int 29

> for (nm in c("coefficients", "residuals", "fitted.values", "rank"))
+     stopifnot(all.equal(lltFit[[nm]], unname(lmFit[[nm]])))
> stopifnot(all.equal(lltFit[["Std. Error"]],
+                     unname(coef(summary(lm(log(Volume) ~ log(Girth), trees)))[,2])))
```

There are several aspects of the C++ code in Figure 6 worth mentioning. The `solve` method for the `LLT` object evaluates, in this case, $(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$ but without actually evaluating the inverse. The calculation of the residuals, $\boldsymbol{y} - \widehat{\boldsymbol{y}}$, can be written, as in R, as `y - fitted`. (But note that **Eigen** classes do not have a "recycling rule as in R. That is, the two vector operands must have the same length.) The `norm()` method evaluates the square root of the sum of squares of the elements of a vector. Although one does not explicitly evaluate $(\boldsymbol{X}'\boldsymbol{X})^{-1}$ one does evaluate $\boldsymbol{L}^{-1}$ to obtain the standard errors. Note also the use of the `colwise()` method in the evaluation of the standard errors. It applies a method to the columns of a matrix, returning a vector. The **Eigen** `colwise()` and `rowwise()` methods are similar in effect to the `apply` function in R.

In the descriptions of other methods for solving least squares problems, much of the code parallels that shown in Figure 6. The redundant parts are omitted, and only the evaluation of the coefficients, the rank and the standard errors is shown. Actually, the standard errors are calculated only up to the scalar multiple of s, the residual standard error, in these code fragments. The calculation of the residuals and s and the scaling of the coefficient standard errors is the same for all methods. (See the files `fastLm.h` and `fastLm.cpp` in the **RcppEigen** source package for details.)

4.2 Least squares using the unpivoted QR decomposition

A QR decomposition has the form

$$\boldsymbol{X} = \boldsymbol{Q}\boldsymbol{R} = \boldsymbol{Q}_1\boldsymbol{R}_1$$

where $\boldsymbol{Q}$ is an $n \times n$ orthogonal matrix, which means that $\boldsymbol{Q}'\boldsymbol{Q} = \boldsymbol{Q}\boldsymbol{Q}' = \boldsymbol{I}_n$, and the $n \times p$ matrix $\boldsymbol{R}$ is zero below the main diagonal. The $n \times p$ matrix $\boldsymbol{Q}_1$ is the first p columns of $\boldsymbol{Q}$ and the $p \times p$ upper triangular matrix $\boldsymbol{R}_1$ is the top p rows of $\boldsymbol{R}$. There are three **Eigen** classes for the QR decomposition:

`HouseholderQR` provides the basic QR decomposition using Householder transformations, `ColPivHouseholderQR` incorporates column pivots and `FullPivHouseholderQR` incorporates both row and column pivots.

Figure 7 shows a least squares solution using the unpivoted QR decomposition.

```
using Eigen::HouseholderQR;

const HouseholderQR<MatrixXd> QR(X);
const VectorXd           betahat(QR.solve(y));
const VectorXd            fitted(X * betahat);
const int                     df(n - p);
const VectorXd                se(QR.matrixQR().topRows(p).
                                 triangularView<Upper>().
                                 solve(MatrixXd::Identity(p,p)).
                                 rowwise().norm());
```

Figure 7: QRLSCpp: Least squares using the unpivoted QR decomposition

The calculations in Figure 7 are quite similar to those in Figure 6. In fact, if one had extracted the upper triangular factor (the `matrixU()` method) from the `LLT` object in Figure 6, the rest of the code would be nearly identical.

4.3 Handling the rank-deficient case

One important consideration when determining least squares solutions is whether rank($\boldsymbol{X}$) is p, a situation described by saying that $\boldsymbol{X}$ has "full column rank". When $\boldsymbol{X}$ does not have full column rank it is said to be "rank deficient".

Although the theoretical rank of a matrix is well-defined, its evaluation in practice is not. At best one can compute an effective rank according to some tolerance. Decompositions that allow to estimation of the rank of the matrix in this way are said to be "rank-revealing".

Because the `model.matrix` function in R does a considerable amount of symbolic analysis behind the scenes, one usually ends up with full-rank model matrices. The common cases of rank-deficiency, such as incorporating both a constant term and a full set of indicators columns for the levels of a factor, are eliminated. Other, more subtle, situations will not be detected at this stage, however. A simple example occurs when there is a "missing cell" in a two-way layout and the interaction of the two factors is included in the model.

```
> dd <- data.frame(f1 = gl(4, 6, labels = LETTERS[1:4]),
+                  f2 = gl(3, 2, labels = letters[1:3]))[-(7:8), ]
> xtabs(~ f2 + f1, dd)                    # one missing cell

   f1
f2  A B C D
  a 2 0 2 2
  b 2 2 2 2
  c 2 2 2 2

> mm <- model.matrix(~ f1 * f2, dd)
> kappa(mm)         # large condition number, indicating rank deficiency

[1] 4.309225e+16

> rcond(mm)         # alternative evaluation, the reciprocal condition number

[1] 2.320603e-17

> (c(rank=qr(mm)$rank, p=ncol(mm))) # rank as computed in R's qr function

rank    p
  11   12
```

```
> set.seed(1)
> dd$y <- mm %*% seq_len(ncol(mm)) + rnorm(nrow(mm), sd = 0.1)
>                         # lm detects the rank deficiency
> fm1 <- lm(y ~ f1 * f2, dd)
> writeLines(capture.output(print(summary(fm1), signif.stars=FALSE))[9:22])

Coefficients: (1 not defined because of singularities)
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.97786    0.05816   16.81 3.41e-09
f1B         12.03807    0.08226  146.35  < 2e-16
f1C          3.11722    0.08226   37.90 5.22e-13
f1D          4.06852    0.08226   49.46 2.83e-14
f2b          5.06012    0.08226   61.52 2.59e-15
f2c          5.99759    0.08226   72.91 4.01e-16
f1B:f2b     -3.01476    0.11633  -25.92 3.27e-11
f1C:f2b      7.70300    0.11633   66.22 1.16e-15
f1D:f2b      8.96425    0.11633   77.06  < 2e-16
f1B:f2c           NA         NA      NA       NA
f1C:f2c     10.96133    0.11633   94.23  < 2e-16
f1D:f2c     12.04108    0.11633  103.51  < 2e-16
```

The `lm` function for fitting linear models in R uses a rank-revealing form of the QR decomposition. When the model matrix is determined to be rank deficient, according to the threshold used in R's QR decomposition, the model matrix is reduced to rank$(\boldsymbol{X})$ columns by pivoting selected columns (those that are apparently linearly dependent on columns to their left) to the right hand side of the matrix. A solution for this reduced model matrix is determined and the coefficients and standard errors for the redundant columns are flagged as missing.

An alternative approach is to evaluate the "pseudo-inverse" of $\boldsymbol{X}$ from the singular value decomposition (SVD) of $\boldsymbol{X}$ or the eigendecomposition of $\boldsymbol{X}'\boldsymbol{X}$. The SVD is of the form

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}' = \boldsymbol{U}_1\boldsymbol{D}_1\boldsymbol{V}'$$

where $\boldsymbol{U}$ is an orthogonal $n \times n$ matrix and $\boldsymbol{U}_1$ is its leftmost p columns, $\boldsymbol{D}$ is $n \times p$ and zero off the main diagonal so that $\boldsymbol{D}_1$ is a $p \times p$ diagonal matrix with non-decreasing non-negative diagonal elements, and $\boldsymbol{V}$ is a $p \times p$ orthogonal matrix. The pseudo-inverse of $\boldsymbol{D}_1$, written $\boldsymbol{D}_1^+$ is a $p \times p$ diagonal matrix whose first $r = \text{rank}(\boldsymbol{X})$ diagonal elements are the inverses of the corresponding diagonal elements of $\boldsymbol{D}_1$ and whose last $p - r$ diagonal elements are zero.

The tolerance for determining if an element of the diagonal of $\boldsymbol{D}$ is considered to be (effectively) zero is a multiple of the largest singular value (i.e. the $(1, 1)$ element of $\boldsymbol{D}$).

In Figure 8 a utility function, `Dplus`, is defined to return the pseudo-inverse as a diagonal matrix, given the singular values (the diagonal of $\boldsymbol{D}$) and the apparent rank. To be able to use this function with the eigendecomposition where the eigenvalues are in increasing order, a Boolean argument `rev` is included indicating whether the order is reversed.

```
using Eigen::DiagonalMatrix;
using Eigen::Dynamic;

inline DiagonalMatrix<double, Dynamic> Dplus(const ArrayXd& D,
                                             int r, bool rev=false) {
    VectorXd   Di(VectorXd::Constant(D.size(), 0.));
    if (rev) Di.tail(r)  = D.tail(r).inverse();
    else Di.head(r)      = D.head(r).inverse();
    return DiagonalMatrix<double, Dynamic>(Di);
}
```

Figure 8: DplusCpp: Create the diagonal matrix $\boldsymbol{D}^+$ from the array of singular values $\boldsymbol{d}$

4.4 Least squares using the SVD

With these definitions the code for least squares using the singular value decomposition can be written as in Figure 9.

```
using Eigen::JacobiSVD;

const JacobiSVD<MatrixXd>
                UDV(X.jacobiSvd(Eigen::ComputeThinU|Eigen::ComputeThinV));
const ArrayXd               D(UDV.singularValues());
const int                   r((D > D[0] * threshold()).count());
const MatrixXd             VDp(UDV.matrixV() * Dplus(D, r));
const VectorXd         betahat(VDp * UDV.matrixU().adjoint() * y);
const int                  df(n - r);
const VectorXd             se(s * VDp.rowwise().norm());
```

Figure 9: **SVDLSCpp**: Least squares using the SVD

In the rank-deficient case this code will produce a complete set of coefficients and their standard errors. It is up to the user to note that the rank is less than p, the number of columns in $\boldsymbol{X}$, and hence that the estimated coefficients are just one of an infinite number of coefficient vectors that produce the same fitted values. It happens that this solution is the minimum norm solution.

The standard errors of the coefficient estimates in the rank-deficient case must be interpreted carefully. The solution with one or more missing coefficients, as returned by the `lm.fit` function in R and by the column-pivoted QR decomposition described in Section 4.6, does not provide standard errors for the missing coefficients. That is, both the coefficient and its standard error are returned as `NA` because the least squares solution is performed on a reduced model matrix. It is also true that the solution returned by the SVD method is with respect to a reduced model matrix but the p coefficient estimates and their p standard errors don't show this. They are, in fact, linear combinations of a set of r coefficient estimates and their standard errors.

4.5 Least squares using the eigendecomposition

The eigendecomposition of $\boldsymbol{X}'\boldsymbol{X}$ is defined as

$$\boldsymbol{X}'\boldsymbol{X} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}'$$

where $\boldsymbol{V}$, the matrix of eigenvectors, is a $p \times p$ orthogonal matrix and $\boldsymbol{\Lambda}$ is a $p \times p$ diagonal matrix with non-increasing, non-negative diagonal elements, called the eigenvalues of $\boldsymbol{X}'\boldsymbol{X}$. When the eigenvalues are distinct this $\boldsymbol{V}$ is the same as that in the SVD. Also, the eigenvalues of $\boldsymbol{X}'\boldsymbol{X}$ are the squares of the singular values of $\boldsymbol{X}$.

With these definitions one can adapt much of the code from the SVD method for the eigendecomposition, as shown in Figure 10.

```
using Eigen::SelfAdjointEigenSolver;

const SelfAdjointEigenSolver<MatrixXd>
                        VLV(MatrixXd(p, p).setZero()
                                          .selfadjointView<Lower>
                                          .rankUpdate(X.adjoint()));
const ArrayXd             D(eig.eigenvalues());
const int                 r((D > D[p - 1] * threshold()).count());
const MatrixXd           VDp(VLV.eigenvectors() * Dplus(D.sqrt(),r,true));
const VectorXd       betahat(VDp * VDp.adjoint() * X.adjoint() * y);
const VectorXd            se(s * VDp.rowwise().norm());
```

Figure 10: SymmEigLSCpp: Least squares using the eigendecomposition

4.6 Least squares using the column-pivoted QR decomposition

The column-pivoted QR decomposition provides results similar to those from R in both the full-rank and the rank-deficient cases. The decomposition is of the form

$$\boldsymbol{X}\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{R} = \boldsymbol{Q}_1\boldsymbol{R}_1$$

where, as before, $\boldsymbol{Q}$ is $n \times n$ and orthogonal and $\boldsymbol{R}$ is $n \times p$ and upper triangular. The $p \times p$ matrix $\boldsymbol{P}$ is a permutation matrix. That is, its columns are a permutation of the columns of $\boldsymbol{I}_p$. It serves to reorder the columns of $\boldsymbol{X}$ so that the diagonal elements of $\boldsymbol{R}$ are non-increasing in magnitude.

An instance of the class `Eigen::ColPivHouseholderQR` has a `rank()` method returning the computational rank of the matrix. When $\boldsymbol{X}$ is of full rank one can use essentially the same code as in the unpivoted decomposition except that one must reorder the standard errors. When $\boldsymbol{X}$ is rank-deficient, the coefficients and standard errors are evaluated for the leading r columns of $\boldsymbol{X}\boldsymbol{P}$ only.

In the rank-deficient case the straightforward calculation of the fitted values, as $\boldsymbol{X}\widehat{\boldsymbol{\beta}}$, cannot be used. One could do some complicated rearrangement of the columns of X and the coefficient estimates but it is conceptually (and computationally) easier to employ the relationship

$$\widehat{\boldsymbol{y}} = \boldsymbol{Q}_1\boldsymbol{Q}_1'\boldsymbol{y} = \boldsymbol{Q}\begin{bmatrix}\boldsymbol{I}_r & \boldsymbol{0}\\ \boldsymbol{0} & \boldsymbol{0}\end{bmatrix}\boldsymbol{Q}'\boldsymbol{y}$$

The vector $\boldsymbol{Q}'\boldsymbol{y}$ is called the "effects" vector in R.

```
using Eigen::ColPivHouseholderQR;
typedef ColPivHouseholderQR<MatrixXd>::PermutationType  Permutation;

const ColPivHouseholderQR<MatrixXd> PQR(X);
const Permutation                   Pmat(PQR.colsPermutation());
const int                              r(PQR.rank());
VectorXd                               betahat, fitted, se;
if (r == X.cols()) { // full rank case
    betahat  = PQR.solve(y);
    fitted   = X * betahat;
    se       = Pmat * PQR.matrixQR().topRows(p).triangularView<Upper>().
        solve(MatrixXd::Identity(p, p)).rowwise().norm();
} else {
    MatrixXd                      Rinv(PQR.matrixQR().topLeftCorner(r, r).
           triangularView<Upper>().
           solve(MatrixXd::Identity(r, r)));
    VectorXd                   effects(PQR.householderQ().adjoint() * y);
    betahat.fill(::NA_REAL);
    betahat.head(r)                    = Rinv * effects.head(r);
    betahat                            = Pmat * betahat;
   // create fitted values from effects
   // (cannot use X * betahat when X is rank-deficient)
    effects.tail(X.rows() - r).setZero();
    fitted                             = PQR.householderQ() * effects;
    se.fill(::NA_REAL);
    se.head(r)                         = Rinv.rowwise().norm();
    se                                 = Pmat * se;
}
```

Figure 11: **ColPivQRLSCpp**: Least squares using the pivoted QR decomposition

Just to check that the code in Figure 11 does indeed provide the desired answer

```
> print(summary(fmPQR <- fastLm(y ~ f1 * f2, dd)), signif.stars=FALSE)
```

```
Call:
fastLm.formula(formula = y ~ f1 * f2, data = dd)

             Estimate Std. Error t value  Pr(>|t|)
(Intercept)  0.977859   0.058165  16.812 3.413e-09
f1B         12.038068   0.082258 146.346 < 2.2e-16
f1C          3.117222   0.082258  37.896 5.221e-13
f1D          4.068523   0.082258  49.461 2.833e-14
f2b          5.060123   0.082258  61.516 2.593e-15
f2c          5.997592   0.082258  72.912 4.015e-16
f1B:f2b     -3.014763   0.116330 -25.916 3.266e-11
f1C:f2b      7.702999   0.116330  66.217 1.156e-15
f1D:f2b      8.964251   0.116330  77.059 < 2.2e-16
f1B:f2c            NA         NA      NA        NA
f1C:f2c     10.961326   0.116330  94.226 < 2.2e-16
f1D:f2c     12.041081   0.116330 103.508 < 2.2e-16

Residual standard error: 0.2868 on 11 degrees of freedom
Multiple R-squared: 0.9999,        Adjusted R-squared: 0.9999
```

```
> all.equal(coef(fm1), coef(fmPQR))
```

```
[1] TRUE
```

```
> all.equal(unname(fitted(fm1)), fitted(fmPQR))
```

```
[1] TRUE
```

```
> all.equal(unname(residuals(fm1)), residuals(fmPQR))
```

```
[1] TRUE
```

The rank-revealing SVD method produces the same fitted values but not the same coefficients.

```
> print(summary(fmSVD <- fastLm(y ~ f1 * f2, dd, method=4L)), signif.stars=FALSE)
```

```
Call:
fastLm.formula(formula = y ~ f1 * f2, data = dd, method = 4L)

             Estimate Std. Error t value  Pr(>|t|)
(Intercept)  0.977859   0.058165  16.812 3.413e-09
f1B          7.020458   0.038777 181.049 < 2.2e-16
f1C          3.117222   0.082258  37.896 5.221e-13
f1D          4.068523   0.082258  49.461 2.833e-14
f2b          5.060123   0.082258  61.516 2.593e-15
f2c          5.997592   0.082258  72.912 4.015e-16
f1B:f2b      2.002847   0.061311  32.667 2.638e-12
f1C:f2b      7.702999   0.116330  66.217 1.156e-15
f1D:f2b      8.964251   0.116330  77.059 < 2.2e-16
f1B:f2c      5.017610   0.061311  81.838 < 2.2e-16
f1C:f2c     10.961326   0.116330  94.226 < 2.2e-16
f1D:f2c     12.041081   0.116330 103.508 < 2.2e-16

Residual standard error: 0.2868 on 11 degrees of freedom
Multiple R-squared: 0.9999,        Adjusted R-squared: 0.9999
```

```
> all.equal(coef(fm1), coef(fmSVD))
```

```
[1] "'is.NA' value mismatch: 0 in current 1 in target"
```

```
> all.equal(unname(fitted(fm1)), fitted(fmSVD))
```

```
[1] TRUE
```

```
> all.equal(unname(residuals(fm1)), residuals(fmSVD))
```

```
[1] TRUE
```

The coefficients from the symmetric eigendecomposition method are the same as those from the SVD

```
> print(summary(fmVLV <- fastLm(y ~ f1 * f2, dd, method=5L)), signif.stars=FALSE)

Call:
fastLm.formula(formula = y ~ f1 * f2, data = dd, method = 5L)

             Estimate Std. Error t value  Pr(>|t|)
(Intercept)  0.977859   0.058165  16.812 3.413e-09
f1B          7.020458   0.038777 181.049 < 2.2e-16
f1C          3.117222   0.082258  37.896 5.221e-13
f1D          4.068523   0.082258  49.461 2.833e-14
f2b          5.060123   0.082258  61.516 2.593e-15
f2c          5.997592   0.082258  72.912 4.015e-16
f1B:f2b      2.002847   0.061311  32.667 2.638e-12
f1C:f2b      7.702999   0.116330  66.217 1.156e-15
f1D:f2b      8.964251   0.116330  77.059 < 2.2e-16
f1B:f2c      5.017610   0.061311  81.838 < 2.2e-16
f1C:f2c     10.961326   0.116330  94.226 < 2.2e-16
f1D:f2c     12.041081   0.116330 103.508 < 2.2e-16

Residual standard error: 0.2868 on 11 degrees of freedom
Multiple R-squared: 0.9999,        Adjusted R-squared: 0.9999

> all.equal(coef(fmSVD), coef(fmVLV))

[1] TRUE

> all.equal(unname(fitted(fm1)), fitted(fmSVD))

[1] TRUE

> all.equal(unname(residuals(fm1)), residuals(fmSVD))

[1] TRUE
```

4.7 Comparative speed

In the **RcppEigen** package the R function to fit linear models using the methods described above is called `fastLm`. It follows an earlier example in the **Rcpp** package which was carried over to both **RcppArmadillo** and **RcppGSL**. The natural question to ask is, "Is it indeed fast to use these methods based on **Eigen**?". To this end, the example provides benchmarking code for these methods, R's `lm.fit` function and the `fastLm` implementations in the **RcppArmadillo** (François, Eddelbuettel, and Bates, 2011) and **RcppGSL** (François and Eddelbuettel, 2011) packages, if they are installed. The benchmark code, which uses the **rbenchmark** (Kusnierczyk, 2010) package, is in a file named `lmBenchmark.R` in the `examples` subdirectory of the installed **RcppEigen** package.

It can be run as

```
> source(system.file("examples", "lmBenchmark.R", package="RcppEigen"))
```

Results will vary according to the speed of the processor, the number of cores and the implementation of the BLAS (Basic Linear Algebra Subroutines) used. (**Eigen** methods do not use the BLAS but the other methods do.)

If Eigen use multiple cores should we no use Goto o another multi core BLAS a well?

Results obtained on a desktop computer, circa 2010, are shown in Table 2

These results indicate that methods based on forming and decomposing $\boldsymbol{X}'\boldsymbol{X}$, (i.e. LDLt, LLt and SymmEig) are considerably faster than the others. The SymmEig method, using a rank-revealing decomposition, would be preferred, although the LDLt method could probably be modified to be rank-revealing. Do bear in mind that the dimensions of the problem will influence the comparative results. Because there are 100,000 rows in $\boldsymbol{X}$, methods that decompose the whole $\boldsymbol{X}$ matrix (all the methods except those named above) will be at a disadvantage.

The pivoted QR method is 1.6 times faster than R's `lm.fit` on this test and provides nearly the same information as `lm.fit`. Methods based on the singular value decomposition (SVD and GSL) are much slower but, as mentioned above, this is caused in part by $\boldsymbol{X}$ having many more rows than columns. The

Table 2: `lmBenchmark` results on a desktop computer for the default size, $100,000 \times 40$, full-rank model matrix running 20 repetitions for each method. Times (Elapsed, User and Sys) are in seconds. The BLAS in use is a single-threaded version of Atlas (Automatically Tuned Linear Algebra System).

Method	Relative	Elapsed	User	Sys
LLt	1.000000	1.227	1.228	0.000
LDLt	1.037490	1.273	1.272	0.000
SymmEig	2.895681	3.553	2.972	0.572
QR	7.828036	9.605	8.968	0.620
PivQR	7.953545	9.759	9.120	0.624
arma	8.383048	10.286	10.277	0.000
lm.fit	13.782396	16.911	15.521	1.368
SVD	54.829666	67.276	66.321	0.912
GSL	157.531377	193.291	192.568	0.640

GSL method from the GNU Scientific Library uses an older algorithm for the SVD and is clearly out of contention.

An SVD method using the Lapack SVD subroutine, `dgesv`, may be faster than the native **Eigen** implementation of the SVD, which is not a particularly fast method of evaluating the SVD.

5 Delayed evaluation

A form of delayed evaluation is used in **Eigen**. That is, many operators and methods do not evaluate the result but instead return an "expression object" that is evaluated when needed. As an example, even though one writes the $\boldsymbol{X}'\boldsymbol{X}$ evaluation using `.rankUpdate(X.adjoint())` the `X.adjoint()` part is not evaluated immediately. The `rankUpdate` method detects that it has been passed a matrix that is to be used in its transposed form and evaluates the update by taking inner products of columns of $\boldsymbol{X}$ instead of rows of $\boldsymbol{X}'$.

Occasionally the method for `Rcpp::wrap` will not force an evaluation when it should. This is at least what Bill Venables calls an "infelicity" in the code, if not an outright bug. In the code for the transpose of an integer matrix shown in Figure 1 we assigned the transpose as a `MatrixXi` before returning it with `wrap`. The assignment forces the evaluation. If this step is skipped, as in Figure 12, an answer with the correct shape but incorrect contents is obtained.

```
using Eigen::Map;
using Eigen::MatrixXi;
const Map<MatrixXi>  A(as<Map<MatrixXi> >(AA));
return wrap(A.transpose());
```

Figure 12: **badtransCpp**: Transpose producing incorrect results

```
> Ai <- matrix(1:6, ncol=2L)
> ftrans2 <- cxxfunction(signature(AA = "matrix"), badtransCpp, "RcppEigen")
> (At <- ftrans2(Ai))
     [,1] [,2] [,3]
[1,]    1    3    5
[2,]    2    4    6
> all.equal(At, t(Ai))
[1] "Mean relative difference: 0.4285714"
```

Another recommended practice is to assign objects before wrapping them for return to R.

6 Sparse matrices

Eigen provides sparse matrix classes. An R object of class `dgCMatrix` (from the **Matrix** (Bates and Maechler, 2011) package) can be mapped as in Figure 13.

```
using Eigen::Map;
using Eigen::MappedSparseMatrix;
using Eigen::SparseMatrix;
using Eigen::VectorXd;

const MappedSparseMatrix<double>  A(as<MappedSparseMatrix<double> >(AA));
const Map<VectorXd>               y(as<Map<VectorXd> >(yy));
const SparseMatrix<double>       At(A.adjoint());
return List::create(_["At"]  = At,
                    _["Aty"] = At * y);
```

Figure 13: sparseProdCpp: Transpose and product with sparse matrices

```
> sparse1 <- cxxfunction(signature(AA = "dgCMatrix", yy = "numeric"),
+                        sparseProdCpp, "RcppEigen")
> data(KNex, package="Matrix")
> rr <- sparse1(KNex$mm, KNex$y)
> stopifnot(all.equal(rr$At, t(KNex$mm)),
+           all.equal(rr$Aty, as.vector(crossprod(KNex$mm, KNex$y))))
```

A sparse Cholesky decomposition is provided in **Eigen** as the `SimplicialCholesky` class. There are also linkages to the **CHOLMOD** code from the **Matrix** package. At present, both of these are regarded as experimental.

Should there be a word abou lme4Eigen and the speedups?

7 Summary

This paper introduced the **RcppEigen** package which provides high-level linear algebra computations as an extension to the R system. **RcppEigen** is based on the modern C++ library **Eigen** which combines extended functionality with excellent performance, and utilizes **Rcpp** to interface R with C++. Several illustrations covered common matrix operations and several approaches to solving a least squares problem—including an extended discussion of rank-revealing approaches. A short example provided an empirical illustration for the excellent run-time performance of the **RcppEigen** package.

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