Higher-Performance R Programming with C++ Extensions

Part 3: Key Rcpp Application Packages

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Part 3: Key Rcpp Application Packages

Overview

As of mid-June 2017, around 1050 packages on CRAN are using Rcpp

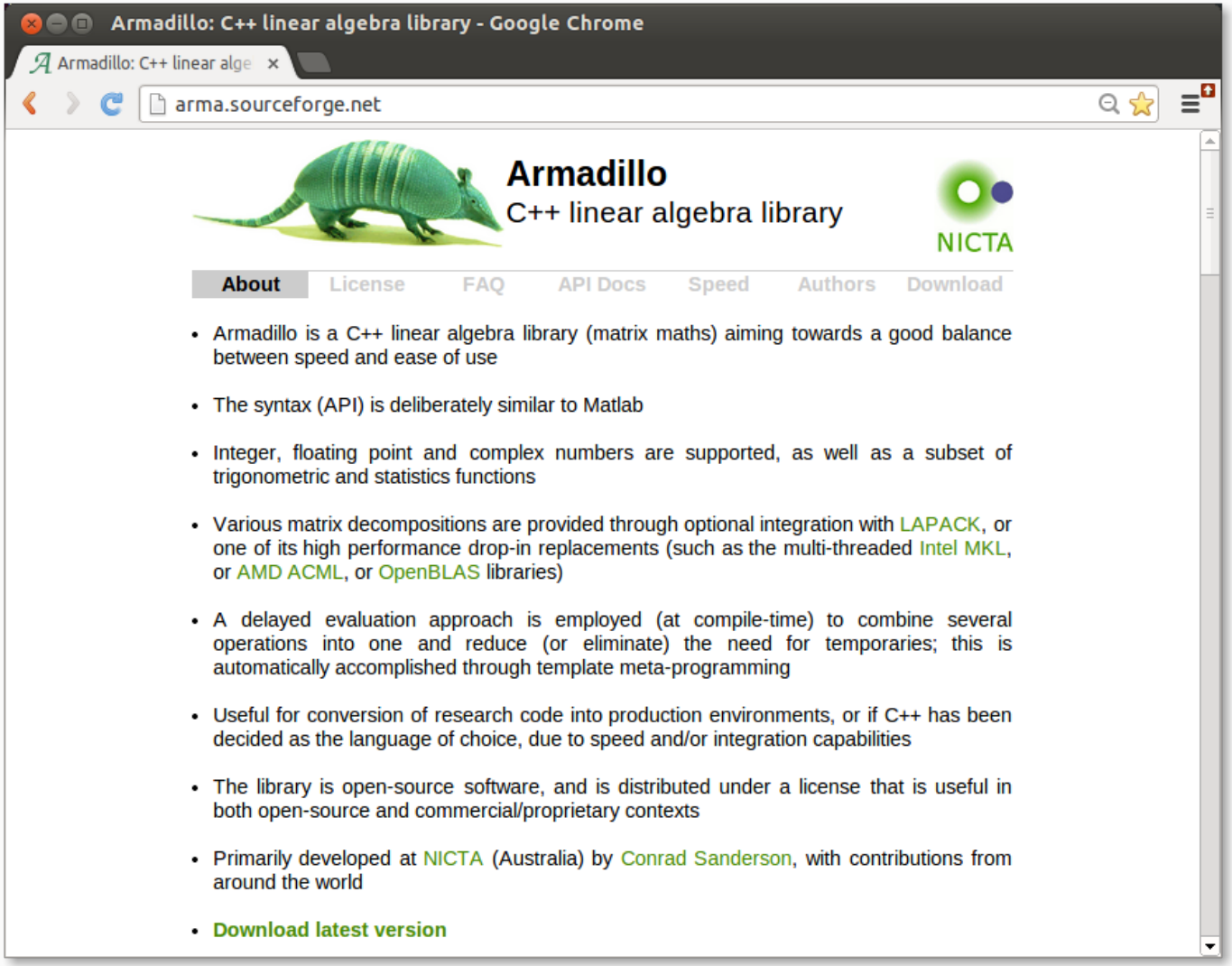
Single biggest "application" is the RcppArmadillo package for linear algebra with around 350

RcppEigen another important package used by around 100 packages including `lme4` and `RStan`

RcppGSL offers vector and matrix classes for the GSL, a popular scientific library

RcppArmadillo

Armadillo


Armadillo: C++ linear algebra library - Google Chrome
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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
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What is Armadillo?

- 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, cubes and fields with all the common operations.
- Very good documentation and examples
    - website,
    - technical report (Sanderson, 2010)
    - CSDA paper (Sanderson and Eddelbuettel, 2014)
    - JOSS paper (Sanderson and Curtin, 2016).
- Modern code, building upon and extending from earlier matrix libraries.
- Responsive and active maintainer, frequent updates.
- Used eg by MLPACK, see 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 to use, just add `LinkingTo: RcppArmadillo, Rcpp` to `DESCRIPTION` (i.e. no added cost beyond Rcpp)
- Really easy from R via Rcpp and automatic converters
- Frequently updated, widely used

Example: Eigen values

```
#include <RcppArmadillo.h>

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

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

Example: Eigen values

```
Rcpp::sourceCpp("code/arma_eigenvalues.cpp")
M <- cbind(c(1,-1), c(-1,1))
getEigenValues(M)
```

```
##      [,1]
## [1,]    0
## [2,]    2
```

```
eigen(M)$values
```

```
## [1] 2 0
```

Example: Vector products

```
#include <RcppArmadillo.h>

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

// another simple example: outer product of a vector,
// returning a matrix
//
// [[Rcpp::export]]
arma::mat rcpparma_outerproduct(const arma::colvec & x) {
    arma::mat m = x * x.t();
    return m;
}

// and the inner product returns a scalar
//
// [[Rcpp::export]]
double rcpparma_innerproduct(const arma::colvec & x) {
    double v = arma::as_scalar(x.t() * x);
    return v;
}
```

FastLm Case Study: Faster Linear Model with FastLm

Background

- Implementations of `fastLm()` have been a staple during development of Rcpp
- First version was in response to a question by Ivo Welch on r-help.
- 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 has since been reimplemented for RcppArmadillo and RcppEigen

Initial FastLm

```
#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
}
```

Newer Version

```
// [[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   );
}
```

Current Version

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

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

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

    double sig2 = arma::as_scalar(arma::trans(resid)*resid/(n-k));
    arma::colvec sterr = arma::sqrt(sig2 *
                                arma::diagvec(arma::pinv(arma::trans(X)*X)));

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

Interface Changes

```
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);
```

Better if performance is a concern. But now RcppArmadillo has efficient `const references` too.

Benchmark

```
edd@don:~$ Rscript ~/git/rcpparmadillo/inst/examples/fastLm.r
                      test replications relative elapsed
3          fLmConstRef(X, y)         5000    1.000   0.245
2          fLmTwoCasts(X, y)         5000    1.045   0.256
4              fLmSEXP(X, y)         5000    1.094   0.268
1           fLmOneCast(X, y)         5000    1.098   0.269
6    fastLmPureDotCall(X, y)         5000    1.118   0.274
8               lm.fit(X, y)         5000    1.673   0.410
5           fastLmPure(X, y)         5000    1.763   0.432
7 fastLm(frm, data = trees)         5000   30.612   7.500
9     lm(frm, data = trees)         5000   30.796   7.545
## continued below
```

Benchmark

```
## continued from above
                     test replications relative elapsed
2       fLmTwoCasts(X, y)        50000    1.000   2.327
3           fLmSEXP(X, y)        50000    1.049   2.442
4       fLmConstRef(X, y)        50000    1.050   2.444
1        fLmOneCast(X, y)        50000    1.150   2.677
6 fastLmPureDotCall(X, y)        50000    1.342   3.123
5        fastLmPure(X, y)        50000    1.988   4.627
7            lm.fit(X, y)        50000    2.141   4.982
edd@don:~$
```

VAR(1) Case Study

Simulating a VAR(1) system of k variables:

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

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

We use $k = 2$ for this example.

VAR(1) in R

```
## parameter and error terms used throughout
a <- matrix(c(0.5,0.1,0.1,0.5),nrow=2)
e <- matrix(rnorm(10000),ncol=2)

## Let's start with the R version
rSim <- function(coeff, errors) {
    simdata <- matrix(0, nrow(errors), ncol(errors))
    for (row in 2:nrow(errors)) {
        simdata[row,] = coeff %*% simdata[(row-1),] +
            errors[row,]
    }
    return(simdata)
}
rData <- rSim(a, e)                    # generated by R
```

VAR(1) in C++

```
arma::mat rcppSim(const arma::mat& coeff,
                  const arma::mat& errors) {
    int m = errors.n_rows;
    int n = errors.n_cols;
    arma::mat simdata(m,n);
    simdata.row(0) = arma::zeros<arma::mat>(1,n);
    for (int row=1; row<m; row++) {
        simdata.row(row) = simdata.row(row-1) * coeff +
            errors.row(row);
    }
    return simdata;
}
```

Benchmark

```
Rcpp::sourceCpp("code/arma_var1.cpp")
rbenchmark::benchmark(rSim(a,e), rcppSim(a, e))[,1:4]
```

```
##             test replications elapsed relative
## 2 rcppSim(a, e)          100   0.023    1.000
## 1    rSim(a, e)          100   1.339   58.217
```

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

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

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

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

MATLAB CODE: kalmanfilter.m

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

  x_prd = A * x_est;                  % Predicted state and covariance
  p_prd = A * p_est * A' + Q;

  S = H * p_prd' * H' + R;            % Estimation
  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;
  y = H * x_est;                      % Compute the estimated measurements
end                                   % of the function
```

MATLAB CODE: kalmanM.m WITH LOOP

```
function Y = kalmanM(pos)
  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 ];    % Initialize measurement matrix
  Q = eye(6);
  R = 1000 * eye(2);
  x_est = zeros(6, 1);                 % x_est=[x,y,Vx,Vy,Ax,Ay]'
  p_est = zeros(6, 6);
  numPts = size(pos,1);
  Y = zeros(numPts, 2);
  for idx = 1:numPts
    z = pos(idx, :)';
    x_prd = A * x_est;                 % Predicted state and covariance
    p_prd = A * p_est * A' + Q;
    S = H * p_prd' * H' + R;           % Estimation
    B = H * p_prd';
    klm_gain = (S \ B)';
    x_est = x_prd + klm_gain * (z - H * x_prd);  % Estimated state and covariance
    p_est = p_prd - klm_gain * H * p_prd;
    Y(idx, :) = H * x_est;             % Compute the estimated measurements
  end
end   % of the function
```

Now in R

```
FirstKalmanR <- function(pos) {
    kalmanfilter <- function(z) {
        dt <- 1
        A <- matrix(c( 1, 0, dt, 0, 0, 0, 0, 1, 0, dt, 0, 0,  # x,  y
                       0, 0, 1, 0, dt, 0, 0, 0, 0, 1, 0, dt,  # Vx, Vy
                       0, 0, 0, 0, 1,  0, 0, 0, 0, 0, 0,  1), # Ax, 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)
        xprd <- A %*% xest          # predicted state and covriance
        pprd <- A %*% pest %*% t(A) + Q
        S <- H %*% t(pprd) %*% t(H) + R     # estimation
        B <- H %*% t(pprd)
        kalmangain <- t(solve(S, B))
        ## estimated state and covariance, assign to vars in parent env
        xest <<- xprd + kalmangain %*% (z - H %*% xprd)
        pest <<- pprd - kalmangain %*% H %*% pprd
        y <- H %*% xest                     # compute the estimated measurements
    }
    xest <- matrix(0, 6, 1)
    pest <- matrix(0, 6, 6)
    N <- nrow(pos)
    y <- matrix(NA, N, 2)
    for (i in 1:N) y[i,] <- kalmanfilter(t(pos[i,,drop=FALSE]))
    invisible(y)
}
```

Improved in R

```
KalmanR <- function(pos) {
    kalmanfilter <- function(z) {
        xprd <- A %*% xest                          # predicted state and covariance
        pprd <- A %*% pest %*% t(A) + Q
        S <- H %*% t(pprd) %*% t(H) + R             # estimation
        B <- H %*% t(pprd)
        kalmangain <- t(solve(S, B))
        xest <<- xprd + kalmangain %*% (z - H %*% xprd)    # est. state and covariance
        pest <<- pprd - kalmangain %*% H %*% pprd          # ass. to vars in parent env
        y <- H %*% xest                             # compute the estimated measurements
    }
    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,] <- kalmanfilter(t(pos[i,,drop=FALSE]))
    invisible(Y)
}
```

And now in C++

```
// [[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) = 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);
    }

   // cont. below
```

And now in C++

```
// continued
    // sole member function: 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, kalmangain;
       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();
           kalmangain = (solve(S, B)).t();
           // estimated state and covariance
           xest = xprd + kalmangain * (z - H * xprd);
           pest = pprd - kalmangain * H * pprd;
           // compute the estimated measurements
           y = H * xest;
           Y.row(i) = y.t();
       }
       return Y;
    }
};
```

And now in C++

And the call:

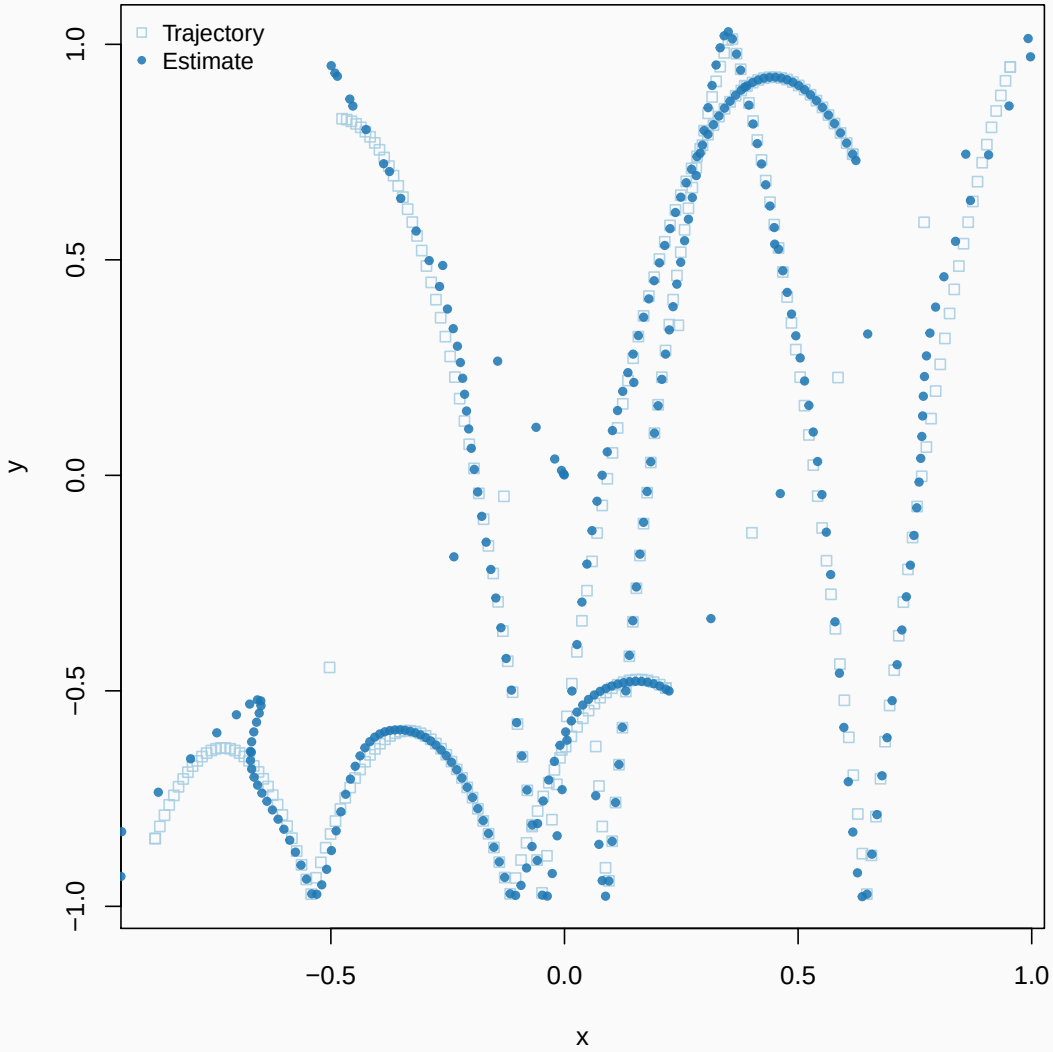
```
// [[Rcpp::export]]
mat KalmanCpp(mat Z) {
  Kalman K;
  mat Y = K.estimate(Z);
  return Y;
}
```

Benchmark

```
library(rbenchmark)
Rcpp::sourceCpp("code/kalman.cpp")
source("code/kalman.R")
p <- as.matrix(read.table("code/pos.txt",
                          header=FALSE,
                          col.names=c("x","y")))
benchmark(KalmanR(p), FirstKalmanR(p), KalmanCpp(p),
          order="relative", replications=500)[,1:4]
```

```
##              test replications elapsed relative
## 3    KalmanCpp(p)          500   3.426    1.000
## 1      KalmanR(p)          500  10.948    3.196
## 2 FirstKalmanR(p)          500  14.388    4.200
```

Reproduced Figure



Sparse Matrix Case Study

A nice example for work on R objects.

```
library(Matrix)
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 Matrix

```
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 Matrix

```
#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 Matrix

```
Rcpp::sourceCpp('code/arma_sparse.cpp')
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
```

RcppEigen

RcppEigen

- RcppEigen wraps the Eigen library for linear algebra.
- Eigen is similar to Armadillo, and very highly optimised—by internal routines replacing even the BLAS for performance.
- Eigen offers a more complete API than Armadillo (but I prefer to work with the simpler Armadillo, most of the time).
- RcppEigen was started by Doug Bates who needed sparse matrix support for his C++ rewrite of lme4.
- Eigen can be faster than Armadillo, eg CRAN package robustHD (using Armadillo) with a drop-in replacement sparseLTSEigen sees gain of 1/4 to 1/3.
- Documented in Bates and Eddelbuettel (JSS, 2013) paper

RcppEigen fastLm

```
// part of larger example showing ability to compute
// model fitting projection via different decompositions

static inline lm do_lm(const Map<MatrixXd> &X, const Map<VectorXd> &y, int type) {
switch(type) {
case ColPivQR_t:
    return ColPivQR(X, y);
case QR_t:
    return QR(X, y);
case LLT_t:
    return Llt(X, y);
case LDLT_t:
    return Ldlt(X, y);
case SVD_t:
    return SVD(X, y);
case SymmEigen_t:
    return SymmEigen(X, y);
case GESDD_t:
    return GESDD(X, y);
}
throw invalid_argument("invalid type");
return ColPivQR(X, y);  // -Wall
}
```

RcppEigen fastLm

```
const Map<MatrixXd>  X(as<Map<MatrixXd> >(Xs));
const Map<VectorXd>  y(as<Map<VectorXd> >(ys));
Index                n = X.rows();

                     // Select and apply the least squares method
lm                  ans(do_lm(X, y, ::Rf_asInteger(type)));

                     // Copy coefficients and install names, if any
NumericVector     coef(wrap(ans.coef()));
List          dimnames(NumericMatrix(Xs).attr("dimnames"));
VectorXd         resid = y - ans.fitted();
int               rank = ans.rank();
int                 df = (rank == ::NA_INTEGER) ? n - X.cols() : n - rank;
double               s = resid.norm() / std::sqrt(double(df));

                     // Create the standard errors
VectorXd             se = s * ans.se();

return List::create(Named("coefficients")  = coef,
                    Named("se")            = se,
                    Named("rank")          = rank,
                    Named("df.residual")   = df,
                    Named("residuals")     = resid,
                    Named("s")             = s,
                    Named("fitted.values") = ans.fitted());
```

RcppEigen fastLm

Doug defines a base class `lm` from which the following classes derive:

- LLt (standard Cholesky decomposition)
- LDLt (robust Cholesky decompostion with pivoting)
- SymmEigen (standard Eigen-decomposition)
- QR (standard QR decomposition)
- ColPivQR (Householder rank-revealing QR decomposition with column-pivoting)
- SVD (standard SVD decomposition)

The example file `lmBenchmark.R` in the package runs through these.

RcppEigen fastLm

```
edd@don:~$ r git/rcppeigen/inst/examples/lmBenchmark.R
lm benchmark for n = 100000 and p = 40: nrep = 20
      test relative elapsed user.self sys.self
8       LLt    1.000   1.749     1.712    0.040
3      LDLt    1.042   1.823     1.776    0.048
6   SymmEig    2.751   4.812     3.964    0.844
7        QR    4.012   7.017     6.044    0.964
1    lm.fit    4.359   7.624    12.308   16.764
2     PivQR    4.523   7.911     6.932    1.128
9      arma    5.719  10.003    15.768   22.080
4     GESDD   10.447  18.272    25.112   31.372
5       SVD   35.584  62.236    59.304    2.952
10      GSL   69.646 121.811   122.168    8.952
edd@don:~$
```

RcppEigen Final Remark

Doug often reminds us about the occassional fine differences between *statistical* numerical analysis and standard numerical analysis.

Pivoting schemes are a good example. R uses a custom decomposition (with pivoting) inside of `lm()` which makes it both robust and precise, particularly for rank-deficient matrices.

The example for `fastLm()` in both RcppArmadillo and RcppEigen provides an illustration.

If you are *really* sure your data is well-behaved, then using a faster (non-pivoting) scheme as in RcppArmadillo is ok.

RcppGSL

RcppGSL

- RcppGSL is a convenience wrapper for accessing the GNU GSL, particularly for vector and matrix functions.
- Given that the GSL is a C library, we need to
  - do memory management – though freeing objects now automatic
  - arrange for the GSL libraries to be found
- RcppGSL may still be a convenient tool for programmers more familiar with C than C++ wanting to deploy GSL algorithms.

GSL Vector Norm Example (older version)

```
#include <RcppGSL.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>

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

// [[Rcpp::export]]
Rcpp::NumericVector colNorm(Rcpp::NumericMatrix NM) {
    // this conversion involves an allocation
    RcppGSL::matrix<double> M = Rcpp::as< RcppGSL::matrix<double> >(NM);
    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 n;                           // return vector
}
```

GSL Vector Norm Example (new version)

```
#include <RcppGSL.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_blas.h>

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

// [[Rcpp::export]]
Rcpp::NumericVector colNorm(const RcppGSL::Matrix & G) {
    int k = G.ncol();
    Rcpp::NumericVector n(k);           // to store results
    for (int j = 0; j < k; j++) {
        RcppGSL::VectorView colview = gsl_matrix_const_column (G, j);
        n[j] = gsl_blas_dnrm2(colview);
    }
    return n;                           // return vector
}
```

GSL Vector Norm Example

```
Rcpp::sourceCpp("code/gslNorm.cpp")
set.seed(42)
M <- matrix(rnorm(25), 5, 5)
colNorm(M)                                  # via GSL
```

```
## [1] 1.70124 2.52644 2.99263 3.90392 2.89203
```

```
apply(M, 2, function(x) sqrt(sum(x^2)))   # via R
```

```
## [1] 1.70124 2.52644 2.99263 3.90392 2.89203
```

GSL bSpline Example

- The example comes from Section 39.7 of the GSL Reference manual, and constructs a data set from the curve $y(x) = \cos(x)\exp(-x/10)$ on the interval $[0, 15]$ with added Gaussian noise — which is then fit via linear least squares using a cubic B-spline basis functions with uniform breakpoints.
- Obviously all this could be done in R too as R can both generate data, and fit models including (B-)splines. But the point to be made here is that we can very easily translate a given GSL program (thanks to RcppGSL), and get it into R with ease thanks to Rcpp and Rcpp attributes.

GSL bSpline Example: C++ (1/6)

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

#include <gsl/gsl_bspline.h>
#include <gsl/gsl_multifit.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_statistics.h>

const int N = 200;                          // number of data points to fit
const int NCOEFFS = 12;                     // number of fit coefficients */
const int NBREAK = (NCOEFFS - 2);           // nbreak = ncoeffs + 2 - k = ncoeffs - 2 since k = 4 */

// [[Rcpp::export]]
Rcpp::List genData() {
    const size_t n = N;
    size_t i;
    double dy;
    gsl_rng *r;
    RcppGSL::Vector w(n), x(n), y(n);
    gsl_rng_env_setup();
    r = gsl_rng_alloc(gsl_rng_default);

    // ...
```

GSL bSpline Example: C++ (2/6)

```
    for (i = 0; i < n; ++i) {
        double xi = (15.0 / (N - 1)) * i;
        double yi = cos(xi) * exp(-0.1 * xi);
        double sigma = 0.1 * yi;
        dy = gsl_ran_gaussian(r, sigma);
        yi += dy;
        x[i] = xi;
        y[i] = yi;
        w[i] = 1.0 / (sigma * sigma);
    }
    gsl_rng_free(r);
    return(Rcpp::DataFrame::create(Rcpp::Named("x") = x,
                                   Rcpp::Named("y") = y,
                                   Rcpp::Named("w") = w));
```

GSL bSpline Example: C++ (3/6)

```
// [[Rcpp::export]]
Rcpp::List fitData(Rcpp::DataFrame D) {
    const size_t ncoeffs = NCOEFFS, nbreak = NBREAK, n = N;
    size_t i, j;
    RcppGSL::Vector y = D["y"];     // access col by name,
    RcppGSL::Vector x = D["x"];     // assign to GSL vectors
    RcppGSL::Vector w = D["w"];
    gsl_bspline_workspace *bw;
    RcppGSL::Vector B(ncoeffs);
    RcppGSL::Vector c(ncoeffs);
    RcppGSL::Matrix X(n, ncoeffs);
    RcppGSL::Matrix cov(ncoeffs, ncoeffs);
    gsl_multifit_linear_workspace *mw;
    double chisq, Rsq, dof, tss;
```

GSL bSpline Example: C++ (4/6)

```
// allocate a cubic bspline workspace (k = 4)
bw = gsl_bspline_alloc(4, nbreak);
mw = gsl_multifit_linear_alloc(n, ncoeffs);
// use uniform breakpoints on [0, 15]
gsl_bspline_knots_uniform(0.0, 15.0, bw);

for (i = 0; i < n; ++i) {       // construct the fit matrix X
    double xi = x[i];
    gsl_bspline_eval(xi, B, bw);    // compute B_j(xi) for all j
    for (j = 0; j < ncoeffs; ++j) { // fill in row i of X
        double Bj = B[j];
        X(i,j) = Bj;
    }
}
```

GSL bSpline Example: C++ (5/6)

```
    gsl_multifit_wlinear(X, w, y, c, cov, &chisq, mw);  // fit
    dof = n - ncoeffs;
    tss = gsl_stats_wtss(w->data, 1, y->data, 1, y->size);
    Rsq = 1.0 - chisq / tss;
    Rcpp::NumericVector FX(151), FY(151);   // smoothed curve
    double xi, yi, yerr;

    for (xi = 0.0, i=0; xi < 15.0; xi += 0.1, i++) {
        gsl_bspline_eval(xi, B, bw);
        gsl_multifit_linear_est(B, c, cov, &yi, &yerr);
        FX[i] = xi;
        FY[i] = yi;
    }
```

GSL bSpline Example: C++ (6/6)

```
    Rcpp::List res =
      Rcpp::List::create(Rcpp::Named("X")=FX,
                         Rcpp::Named("Y")=FY,
                         Rcpp::Named("chisqdof")=
                                  Rcpp::wrap(chisq/dof),
                         Rcpp::Named("rsq")=Rcpp::wrap(Rsq));
    gsl_bspline_free(bw);
    gsl_multifit_linear_free(mw);
    return(res);
}
```

GSL bSpline Example

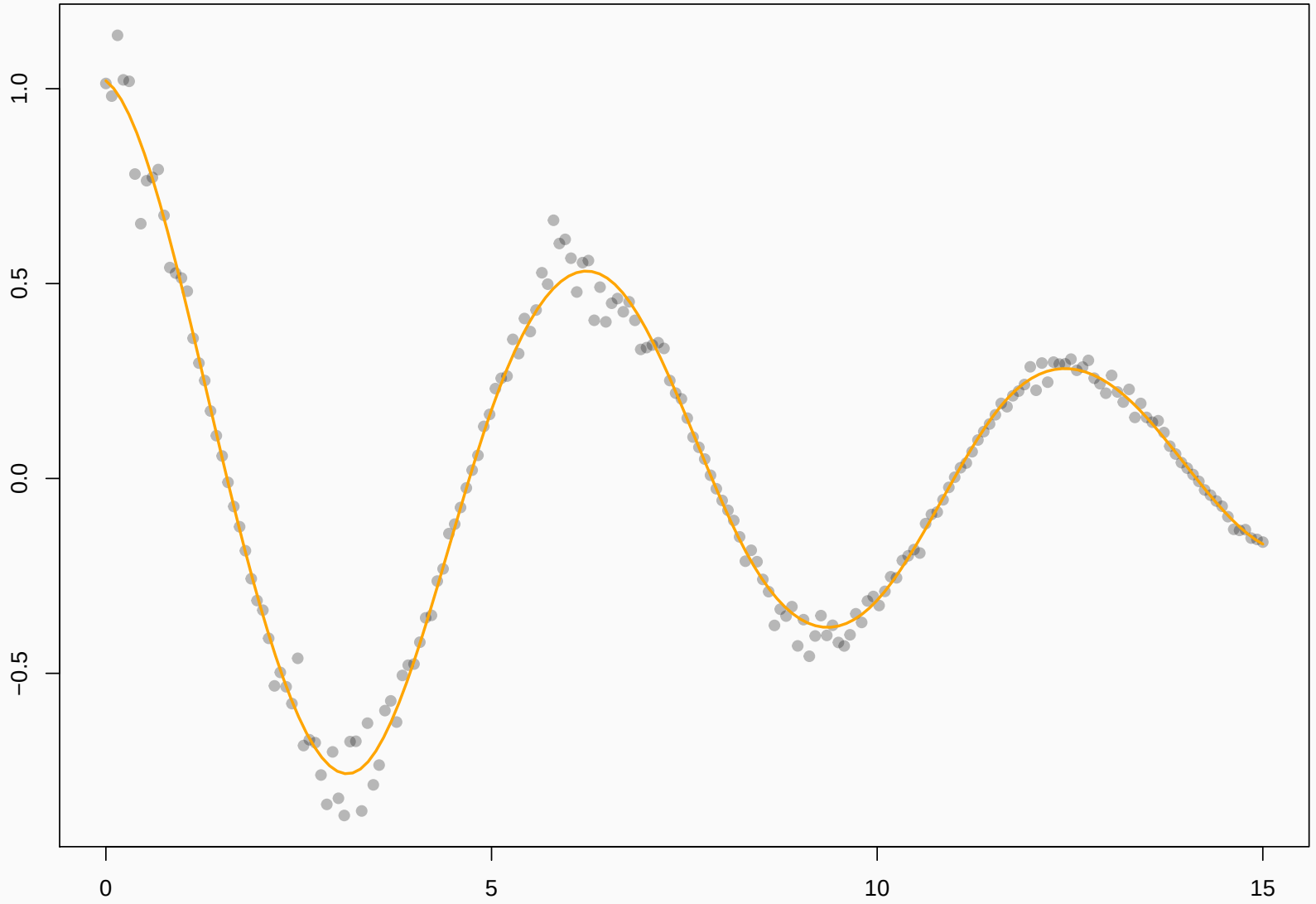
```
Rcpp::sourceCpp("bSpline.cpp")

dat <- genData()                    # generate the data
fit <- fitData(dat)                 # fit the model

X <- fit["X"]]                      # extract vectors
Y <- fit["Y"]]

par(mar=c(3,3,1,1))
plot(dat,"x"], dat,"y"], pch=19, col="#00000044")
lines(X, Y, col="orange", lwd=2)
```

GSL bSpline Example



RcppMLPACK

Overview

Among the 1000+ CRAN packages using Rcpp, several wrap Machine Learning libraries.

Here are three:

- RcppShark based on Shark
- RcppMLPACK based on MLPACK
- dlib based on DLib

MLPACK

High-level:

- Written by Ryan Curtin et al, Georgia Tech
- Uses Armadillo, and like Armadillo, “feels right”
- Qiang Kou created ‘RcppMLPACK v1’, it is on CRAN
- “Simple” packaging by embedding, copy of MLPACK now stale

MLPACK ‘v2’

High-level:

- A few of us are trying to update RcppMLPACK to ‘v2’
- Instead of embedding, amd external library is used
- This makes deployment a little tricker on Windows and macOS
- MLPACK uses Boost, this created issues with (older) RStudio builds

List of Algorithms:

- Collaborative filtering (with many decomposition techniques)
- Decision stumps (one-level decision trees)
- Density estimation trees
- Euclidean minimum spanning tree calculation
- Gaussian mixture models
- Hidden Markov models
- Kernel Principal Components Analysis (optionally with sampling)
- k-Means clustering (with several accelerated algorithms)
- Least-angle regression (LARS/LASSO)
- Linear regression (simple least-squares)
- Local coordinate coding
- Locality-sensitive hashing for approximate nearest neighbor search
- Logistic regression
- Max-kernel search
- Naive Bayes classifier
- Nearest neighbor search with dual-tree algorithms
- Neighborhood components analysis
- Non-negative matrix factorization
- Perceptrons
- Principal components analysis (PCA)
- RADICAL (independent components analysis)
- Range search with dual-tree algorithms
- Rank-approximate nearest neighbor search
- Sparse coding with dictionary learning

RcppMLPACK: K-Means Example

```
#include "RcppMLPACK.h"

using namespace mlpack::kmeans;
using namespace Rcpp;

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

// [[Rcpp::export]]
List cppKmeans(const arma::mat& data, const int& clusters) {

    arma::Col<size_t> assignments;
    KMeans<> k;     // Initialize with the default arguments.
    k.Cluster(data, clusters, assignments);

    return List::create(Named("clusters") = clusters,
                        Named("result")   = assignments);
}
```

Timing

Table 1: Benchmarking result

test	replications	elapsed	relative	user.self	sys.self
mlKmeans(t(wine), 3)	100	0.028	1.000	0.028	0.000
kmeans(wine, 3)	100	0.947	33.821	0.484	0.424

Table taken 'as is' from RcppMLPACK vignette.

RcppMLPACK: Linear Regression Example

```
#include <RcppMLPACK.h>                  // MLPACK, Rcpp and RcppArmadillo

// particular algorithm used here
#include <mlpack/methods/linear_regression/linear_regression.hpp>

// [[Rcpp::export]]
Rcpp::List linearRegression(arma::mat& matX,
                            arma::vec& vecY,
                            const double lambda = 0.0,
                            const bool intercept = true) {

    matX = matX.t();
    mlpack::regression::LinearRegression lr(matX, vecY, lambda, intercept);
    arma::vec parameters = lr.Parameters();
    arma::vec fittedValues(vecY.n_elem);
    lr.Predict(matX,  fittedValues);

    return Rcpp::List::create(Rcpp::Named("parameters") = parameters,
                              Rcpp::Named("fitted") = fittedValues);
}
```

RcppMLPACK: Linear Regression Example

```
suppressMessages(library(utils))
library(RcppMLPACK)
data("trees", package="datasets")
X <- with(trees, cbind(log(Girth), log(Height)))
y <- with(trees, log(Volume))
lmfit <- lm(y ~ X)
# summary(fitted(lmfit))

mlfit <- with(trees, linearRegression(X, y))
# summary(mlfit)

all.equal(unname(fitted(lmfit)),  c(mlfit[["fitted"]]))
```

```
## [1] TRUE
```

RcppMLPACK: Logistic Regression Example

```
#include <RcppMLPACK.h>             // MLPACK, Rcpp and RcppArmadillo
#include <mlpack/methods/logistic_regression/logistic_regression.hpp>   // algo use here

// [[Rcpp::export]]
Rcpp::List logisticRegression(const arma::mat& train, const arma::irowvec& labels,
                              const Rcpp::Nullable<Rcpp::NumericMatrix>& test = R_NilValue) {

    // MLPACK wants Row<size_t> which is an unsigned representation that R does not have
    arma::Row<size_t> labelsur, resultsur;

    // TODO: check that all values are non-negative
    labelsur = arma::conv_to<arma::Row<size_t>>::from(labels);

    // Initialize with the default arguments. TODO: support more arguments>
    mlpack::regression::LogisticRegression<> lrc(train, labelsur);
    arma::vec parameters = lrc.Parameters();

    Rcpp::List return_val;
    if (test.isNotNull()) {
        arma::mat test2 = Rcpp::as<arma::mat>(test);
        lrc.Classify(test2, resultsur);
        arma::vec results = arma::conv_to<arma::vec>::from(resultsur);
        return_val = Rcpp::List::create(Rcpp::Named("parameters") = parameters,
                                        Rcpp::Named("results") = results);
    } else {
        return_val = Rcpp::List::create(Rcpp::Named("parameters") = parameters);
    }
    return return_val;
}
```

RcppMLPACK: Linear Regression Example

```
suppressMessages(library(utils))
library(RcppMLPACK)
example(logisticRegression)
```

```
##
## lgstcR> data(trainSet)
##
## lgstcR> mat <- t(trainSet[, -5])     ## train data, transpose and removing class labels
##
## lgstcR> lab <- trainSet[, 5]         ## class labels for train set
##
## lgstcR> logisticRegression(mat, lab)
## $parameters
## [1] -11.0819909  13.9022481   0.8034972  -9.3485217 -13.0869968
##
##
## lgstcR> testMat <- t(testSet[, -5])  ## test data
##
## lgstcR> logisticRegression(mat, lab, testMat)
## $parameters
## [1] -11.0819909  13.9022481   0.8034972  -9.3485217 -13.0869968
##
## $results
## [1] 0 0 0 1 1 1 1
```

RcppMLPACK: Nearest Neighbors Example

```
#include "RcppMLPACK.h"

using namespace Rcpp;
using namespace mlpack;           using namespace mlpack::neighbor;
using namespace mlpack::metric;   using namespace mlpack::tree;

// [[Rcpp::depends(RcppMLPACK)]]
// [[Rcpp::export]]
List nn(const arma::mat& data, const int k) {
    // using a test from MLPACK 1.0.10 file src/mlpack/tests/allknn_test.cpp
    CoverTree<LMetric<2>, FirstPointIsRoot,
              NeighborSearchStat<NearestNeighborSort> > tree =
        CoverTree<LMetric<2>, FirstPointIsRoot,
                  NeighborSearchStat<NearestNeighborSort> >(data);

    NeighborSearch<NearestNeighborSort, LMetric<2>,
                   CoverTree<LMetric<2>, FirstPointIsRoot,
                             NeighborSearchStat<NearestNeighborSort> > >
        coverTreeSearch(&tree, data, true);

    arma::Mat<size_t> coverTreeNeighbors;
    arma::mat coverTreeDistances;
    coverTreeSearch.Search(k, coverTreeNeighbors, coverTreeDistances);

    return List::create(Named("clusters") = coverTreeNeighbors,
                        Named("result")   = coverTreeDistances);

}
```