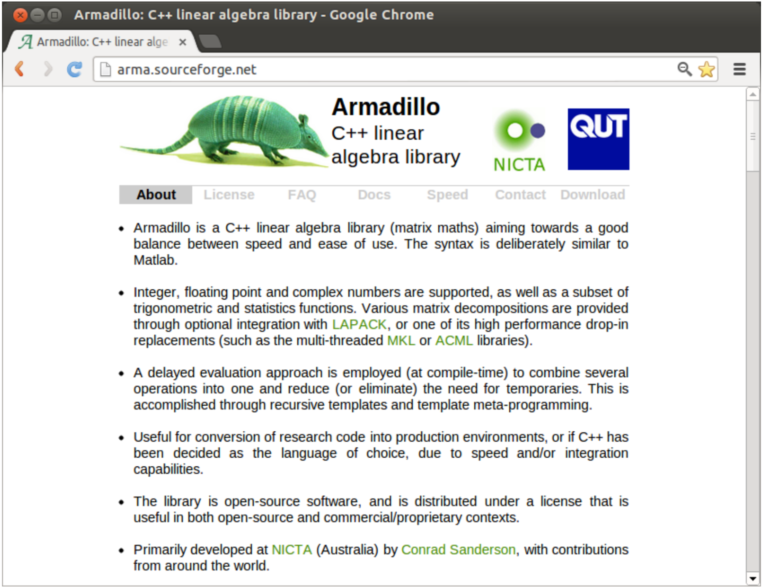
RcppArmadillo: Accelerating R with C++ Linear Algebra

Dr. Dirk Eddelbuettel
edd@debian.org
dirk.eddelbuettel@R-Project.org

Presentation at R/Finance 2013
University of Illinois at Chicago
18 May 2013

Outline

Armadillo



Armadillo: C++ linear algebra library - Google Chrome

arma.sourceforge.net

Armadillo
C++ linear algebra library

NICTA QUT

About License FAQ Docs Speed Contact Download

- 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, 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 MKL or ACML 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 accomplished through recursive templates and 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.

What is Armadillo?

From `arma.sf.net` and slightly edited

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

Integer, floating point and complex numbers are supported, as well as a subset of trigonometric and statistics functions. Various matrix decompositions are provided [...]

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.

The library is open-source software, and is distributed under a license that is useful in both open-source and commercial/proprietary contexts.

What is Armadillo?

From `arma.sf.net` and slightly edited

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

***Integer, floating point and complex numbers** are supported, as well as a subset of trigonometric and statistics functions. **Various matrix decompositions** are provided [...]*

*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.*

*The library is **open-source software**, and is distributed under a license that is useful in both open-source and commercial/proprietary contexts.*

Armadillo highlights

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

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**
- Frequently updated, easy to use

Well-know packages using Rcpp / RcppArmadillo

To name just a few:

- **Amelia** by Gary King et al: Multiple Imputation from cross-section, time-series or both;
- **forecast** by Rob Hyndman et al: Time-series forecasting including state space and automated ARIMA modeling;
- **rugarch** by Alexios Ghalanos: Sophisticated financial time series models;
- **gRbase** by Søren Højsgaard: Graphical modeling

Outline

Armadillo Eigenvalues

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

```
#include <RcppArmadillo.h>

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

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

Armadillo Eigenvalues

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

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

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


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

Multivariate Normal RNG Draw

See
http://gallery.rcpp.org/articles/simulate-multivariate-normal/

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

using namespace Rcpp;

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

Complete file for fastLM

RcppArmadillo src/fastLm.cpp

```
#include <RcppArmadillo.h>

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

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

    arma::colvec coef = arma::solve(X, y);        // fit model y ~ X
    arma::colvec 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
}
```

fastLm using Armadillo

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

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

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

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

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

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

fastLm using Armadillo

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

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

// [[Rcpp::export]]
List fastLm2(colvec y, mat X) {
   int n = X.n_rows, k = X.n_cols;

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

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

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

One note on direct casting with Armadillo

The code as just shown:

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

is very convenient, but does incur an additional copy of each object. A lighter variant uses two steps in which only a pointer to the object 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);
```

If performance is a concern, the latter approach may be preferable.

Outline

Kalman Filter

The Mathworks site has a nice and short example of a classic 'object tracking' problem.

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

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

Kalman Filter: In R

Easy enough – first naive solution

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

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

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

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

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

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

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

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

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

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

  invisible(y)
}
```

Kalman Filter: In R

Easy enough – with some minor refactoring

```
KalmanR <- function(pos) {

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

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

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

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

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

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

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

Kalman Filter: In C++

Using a simple class

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

using namespace arma;

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

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

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

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

Kalman Filter in C++

Trivial to use from R

Given the code from the previous slide, we just add

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

Kalman Filter: Performance

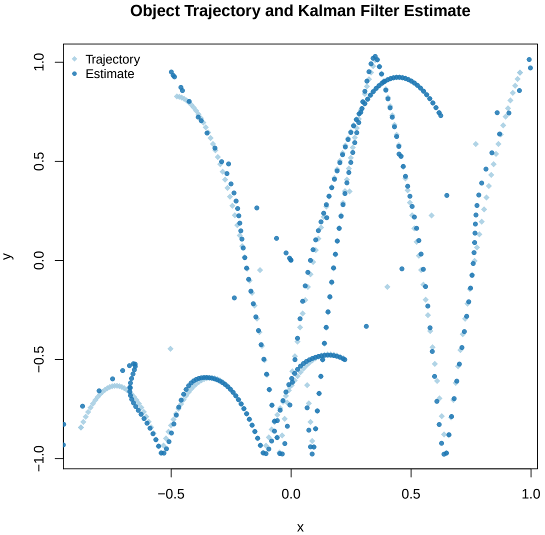
Quite satisfactory relative to R

Even byte-compiled 'better' Rversion is 66 times slower:

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

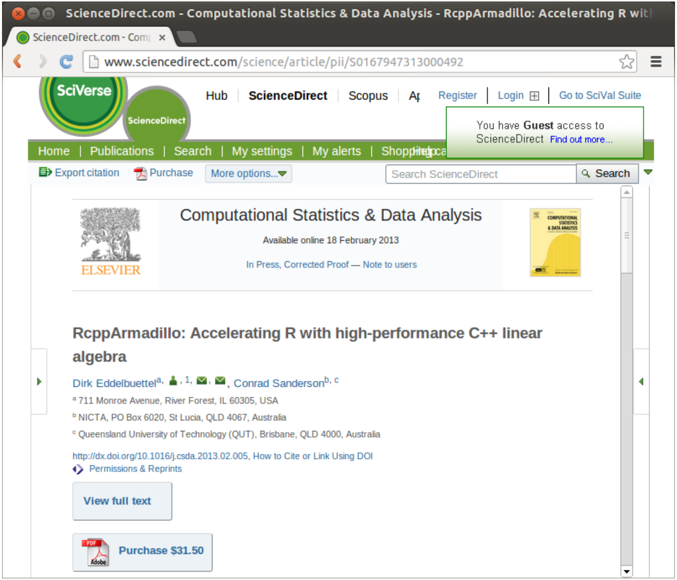
Kalman Filter: Figure

Last but not least we can redo the plot as well

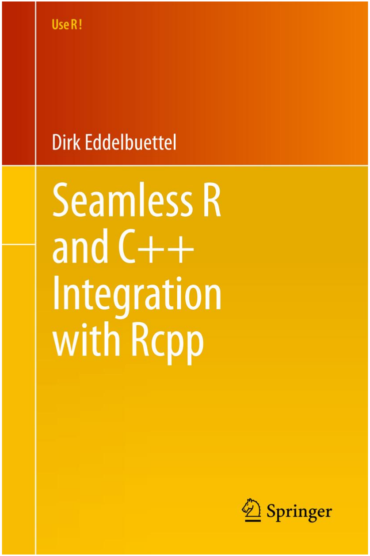


Outline

RcppArmadillo Paper



The Rcpp book



Intially expected in May 2013.
Real Soon Now.

The C in Rcpp stands for ...