Introduction

Timings : Ungrouped

Timings: Grouped

Functions

Speeding up R for Calculating Euclidean Distances

Gibril

Introduction

The task is to calculate euclidean distances between rows in a matrix. It is divided into two subproblems, one with groups and without groups. The following `R` packages have been used:

- `Rcpp`
- `microbenchmark` : for timings

A base `R` function was used as a benchmark for the timings. Three `C` source codes were used which were sourced into `R` via it's `C` API and a `C++` script via `Rcpp` library.

Function	Language
naive_dist	`R`
dot_dist	`R`
fastdist2	`C++`
eucDist	`C` & `R`
r_euc_dist	`C` & `R`
cDist	`C` & `R`

Timings : Ungrouped

Below are sample outputs from the functions for a matrix with 2000 entries for the ungrouped problem and relative timings of each of the functions for different matrix sizes. All timings were in milliseconds.

```
Unit: milliseconds
          expr        min         lq       mean     median         uq
 naive_dist(M) 115.139840 120.060930 130.419957 125.704581 132.208132
       dist(M)   2.432668   3.308361   6.356756   3.926424   5.074132
 r_euc_dist(M)   2.616436   3.330798   7.379464   3.833894   4.486725
   dot_dist(M) 673.753718 723.242430 768.162506 753.764015 796.262480
  fastdist2(M)  10.874602  12.146634  17.410744  13.472862  15.964630
    eucDist(M)   2.605100   3.456320   6.764453   3.846511   4.416576
      cDist(M)   1.877975   2.455699   6.573165   3.195958   3.880205
        max neval
  197.57561   100
   55.02963   100
   52.26835   100
 1017.22427   100
   59.76397   100
   52.69272   100
   54.42619   100
```

```
[1] "naive_dist"
```

```
[1]  8.104245 20.166204 24.063068 14.315379 28.043333 11.600828
```

```
[1] "dist"
```

```
[1]  8.104245 20.166204 24.063068 14.315379 28.043333 11.600828
```

```
[1] "r_euc_dist"
```

```
[1]  8.104245 20.166204 24.063068 14.315379 28.043333 11.600828
```

```
[1] "dot_dist"
```

```
[1]  8.104245 20.166204 24.063068 14.315379 28.043333 11.600828
```

```
[1] "fastdist2"
```

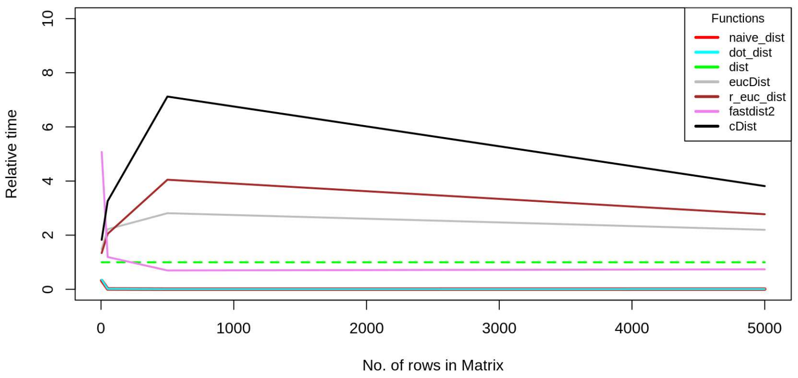
```
[1]  8.104245 20.166204 24.063068 14.315379 28.043333 11.600828
```

```
[1] "eucDist"
```

```
[1]  8.104245 20.166204 24.063068 14.315379 28.043333 11.600828
```

```
[1] "cDist"
```

```
[1]  8.104245 20.166204 24.063068 14.315379 28.043333 11.600828
```



Timings: Grouped

Output

Below are sample outputs from the functions `dist`, `cDist`, `naive_dist`, `r_euc_dist` and `eucDist` for the grouped problem. The outputs from all the functions are the same so only one is shown. The functions `dot_dist` and `fastdist2` could not be modified to allow for a vectorised calculation of distances within each group.

```
INDICES: 1
  [1] 17.953014 29.055633 20.280481 36.992981 30.461330 13.499654 25.497846
  [8] 23.251852  6.954638 16.455878 25.955105 25.275923 31.722903  4.423357
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 [57] 37.957892 40.858410 21.349812 21.089434 53.301610  8.157001  7.588540
 [64] 30.933881 18.090438 24.649020  5.776565 29.720994 15.778034 17.257108
 [71]  5.756167  7.004466 12.595475 20.521479 21.068989 30.803808 29.225970
 [78] 27.347882  2.349000 36.501819 11.637599 17.158372 14.240403 48.986535
 [85] 34.087414 20.143698 38.627851 45.686806 32.519508 25.860807 38.994485
 [92] 33.242297  9.876369 44.173504 48.891321 23.299129 32.791032 63.246715
 [99] 19.402523 15.676941 39.989178 20.257810 23.948055 29.642258 34.587270
[106] 18.595866 12.031678 24.786872 27.948018  6.199463 39.863651 42.035636
[113] 24.577264 19.563353 53.372232  8.353472 10.237007 27.838746 36.742003
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[148] 21.764781 28.033662 37.462474 34.310834 29.039445 41.781881 18.829433
[155] 18.324429 26.853645 33.795420  4.588265 32.069956 51.108088 20.880775
[162] 14.816763  9.813387 21.035600 21.935863 25.916068 10.309388 29.596191
[169] 16.185385 13.461859 23.894291 16.800369 24.629930 21.307082 22.975012
[176] 20.584030 24.261555 22.644066 20.116445 36.058097 23.696190 17.371455
[183] 33.491747 16.918318 19.264459 26.792544 30.180154  6.659574  7.474232
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```

```
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 [97] 18.9441433 25.2930757 17.2031901 18.7183711  3.7107038 22.4090067
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```

```
 [73] 16.9163478 11.0154663 11.6839607 22.3880203 15.8594851  3.0805736
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 [22] 34.269936  9.691621  4.867070 25.357890 23.470902 24.785717 28.261851
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[120] 21.916120
```
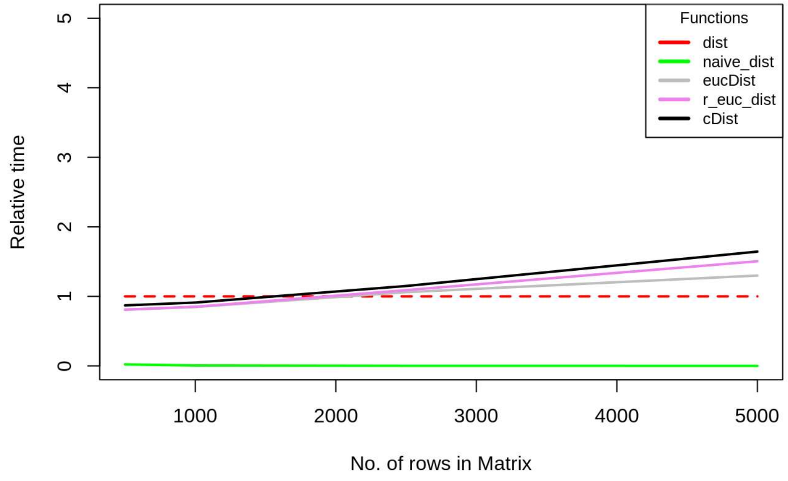

Relative times

The graph below shows the relative timings of each of the functions for different matrix sizes. All timings are in milliseconds.



Functions

The function `naive_dist()` is written purely in R using the formula `dist = sqrt((xi-xj)^2 + (yi-yj)^2)`, `dist()` is the base `R` implementation, `dot_dist()` is also written purely R but uses the dot product method of calculating distances, `fastdist2()` is a `C++` implementation of the calculation and `r_euc_dist()`, `eucDist()` and `cDist` are `R` wrapper functions for `C` implementaions of the calculation.

`naive_dist()`

```
naive_dist <- function(x){

#TODO: function documentation

    result = vector('numeric', length = nrow(x) * (nrow(x) - 1)/2)
    k = 1
    for (i in 1:(nrow(x)-1)){
        for (j in (i+1):nrow(x)){
          result[k] = sqrt((x[i,1]-x[j,1])^2 + (x[i,2] - x[j,2])^2)
          k = k + 1
        }
    }
    result
}
```

dot_dist()

```
dot_dist <- function(x){
# TODO: function documentation
  result = vector('numeric', length = nrow(x) * (nrow(x) - 1)/2)

  i = 1
  m = 1
  while (i <= (nrow(x)-1)){
    for (j in (i+1):nrow(x)){
      k         = x[i,] - x[j,]
      result[m] = sqrt(k %*% k)
      m         = m + 1
    }
    i = i + 1
  }
  result
}
```

fastdist2()

```
// filename: fastdist2.cpp

#include <Rcpp.h>
using namespace Rcpp;

//[[Rcpp::export]]

NumericVector fastdist2 (const NumericMatrix &x){
    unsigned int outrows = x.nrow(), i = 0, j = 0, k = 0;

    Rcpp::NumericVector out(outrows * (outrows - 1)/2);

    for (i = 0; i <= outrows - 2; i++){
        for (j = i+1; j <= outrows - 1; j++){

            out(k) = sqrt(sum(pow(x.row(i) - x.row(j), 2.0)));
                    k++;
}
    }
    return out;
}
```

r_euc_dist() and euc_dist()

```
# filename: r_euc_dist.R
# last edited: 7-AUG-2019


r_euc_dist <- function(matrix, cols_interest = 1:2){

# R wrapper function for euc_dist.c
# check euc_dist.c for source code and function documentation
# input:
#       matrix: an N by 2 numeric matrix
#       cols_interest : if input is a data.frame, the cols to be used.

# output: a vector of euclidean distances between rows
    cpMat   = matrix[, cols_interest]
    len_mat = dim(cpMat)[1] * dim(cpMat)[2]
    n_rows  = nrow(cpMat)
    vec     = as.vector(t(cpMat))

    .C("euc_dist",
       as.double(vec),
       as.integer(len_mat),
       as.double(vector("double", n_rows * (n_rows - 1)/2)))[[3]]

    }

/*
filename: euc_dist.c
last edited: 23-JUL-2019
*/


#include <R.h>
#include <math.h>

/*
Calculates the euclidean distance between rows of a matrix

input:
    vec: a one dimensional array of length N * 2 where N is the number of rows
       in the input matrix.
    len_vec: N * 2
output:
    result: a one dimensional array of length N * 2 containing the calculated distance
s
*/

void euc_dist(double *vec, int *len_vec, double *result)
{
    int k = 0, i, j, iter1 = *len_vec - 3, iter2 = *len_vec - 1;

    for (i = 0; i < iter1; i += 2){
        for (j = i + 2; j < iter2; j += 2){
            result[k] = sqrt((vec[i] - vec[j]) * (vec[i] - vec[j])
                        + (vec[i+1] - vec[j+1]) * (vec[i+1] - vec[j+1]));
            k++;
        }
      }

}
```

eucDist() and eucDist()

```
# filename: eucDist.R
# wrapper function for eucDist.c
# TODO: error correcting code

eucDist <- function(matrix, cols_interest = 1:2){

    cpMat   = matrix[, cols_interest]
    len_mat = dim(matrix)[1] * dim(matrix)[2]
    n_rows  = nrow(matrix)
    n_cols  = ncol(matrix)
    vec     = as.vector(t(matrix))


    .C('eucDist',
       as.double(vec),
       as.integer(n_rows),
       as.integer(n_cols),
       as.double(vector("double", n_rows * (n_rows - 1)/2))
       )[[4]]
}

#include <math.h>
#include <R.h>
#include <Rinternals.h>

/* Euclidean distance */
/*q=.C("eucdist",as.integer(c(1,2,3,4,5,6,7,8)),as.integer(4),as.integer(2),as.double
(vector("double",6))*/
void eucDist(double *x, int *m, int *n, double *d)
{
  /* Arguement:
    1.  x is a matrix of dimension n by m
    2.  m is the number of rows
    3.  n is the number of coloums
    4.  d is the pointer for output */
  /*
   d = sqrt(sum((XI-XJ).^2,2));            % Euclidean
   */
  int i,j,k; /* **pointer; /* Indexers */
  int local_m, local_n;
  local_m = *m, local_n = *n;
  double theSum; /* size_t is an unsigned integer of size 16 bits */
  /*
  XI for indexing rows
  XJ for indexing columns
  XI0 unknown for now
  */
  int  XI, XJ, XI0, index; /* pointers as row indexers*/
  // d = malloc( local_m*(local_m - 1)/2);
  // XI0 =  (double *) x; /* we are not tuching x but using its memory address as XI
*/
  // x = (double) x;
  index = 0;
  for (i=0; i<local_m-1; ++i) { /* Iterating through the rows of the matrix */
    // XI0 =  XI; /* taking the memory address of the array (Refer to line 29) */
    XI = i*local_n; /* Move along memory by n ( the first coloumn */
    XI0 = XI;
    // Rprintf("XI is %d\n", XI);
    for (j=i+1; j<local_m; ++j) { /* iterating through the rows from the i_th row*/
      // XI = x + i*(*n); /* Change to XI happpens here after using it on line 28*/
      XJ = j*local_n;
      // Rprintf("XJ is %d\n", XJ);
      // XI = XI0; /* Index? */
      theSum = 0.0;
      for (k=0;k<local_n;k++,++XI,++XJ){
        theSum += pow((x[XI]- x[XJ]), 2.0);
        // Rprintf("x[XI] is %lf and x[XJ] is %lf\n", x[XI], x[XJ]);
        // Rprintf("The sum is %lf\n", theSum);
        // Rprintf("The sum is %d\n", theSum);
      }
      XI = XI0;
      d[index++] = sqrt(theSum);
      // Rprintf("d is %lf\n", d[index]);
      // XI = XI0; /* Index? */
    }
  }
}
```

cDist() and cDist()

```
/*
filename: cDist.c
last edited: 24-JUL-19
*/


/*
 exactly as euc_dist.c but modified to use R's .Call() interface

 input:
    Rvec: a one-dimensional array of length N * 2 where N is the number of rows
          in the input matrix.

    resLen: an integer (coerced to double) of the number of pairs
            calculated as N * (N - 1)/2.
 output:
    result: a one-dimensional array containing the calculated distances.
*/

#include <R.h>
#include <Rinternals.h>
#include <math.h>

SEXP cDist(SEXP Rvec, SEXP resLen){
    int k = 0, i, j, iter1 = length(Rvec) - 3, iter2 = length(Rvec) - 1;

    SEXP result = PROTECT(allocVector(REALSXP, asReal(resLen)));
    double *vec = REAL(Rvec);

    for(i = 0; i < iter1; i += 2){
        for(j = i + 2; j < iter2; j += 2){
            REAL(result)[k] = sqrt(((vec[i] - vec[j]) * (vec[i] - vec[j])) +
                         ((vec[i+1] - vec[j+1]) * (vec[i+1] - vec[j+1])));
            k++;
        }
    }

    UNPROTECT(1);
    return result;

}

# filename: cDist.R
# last edited: 7-AUG-19


# wrapper function for cDist.c
# see cDist.c for function documentation
#
# input:
#       matrix: an N by 2 numeric matrix
#       cols_interest : if input is a data.frame, the cols to be used.
#
```

```
# output: a vector of euclidean distances between the rows of the matrix.
# TODO: error-correcting code



cDist <- function(matrix, cols_interest = 1:2){
    cpMat  = matrix[, cols_interest]
    vec    = as.vector(t(cpMat))
    reslen = nrow(cpMat) * (nrow(cpMat) - 1) * 0.5

    .Call("cDist",
           as.double(vec),
           as.double(reslen))
}
```