Faster Computation with XPtr

Kisung You

2020-01-30

The function SAMC helps users to build a SAMC sampler easily. However, the main part of our implementation requires numerous evaluations of an energy function at each iteration, which becomes a critical bottleneck in computational aspect. SAMCPLUS exploits a generic framework for passing user-provided C++ functions to our backend. We will use two-dimensional multimodal example to introduce details on how to boost your computation using XPtr.

Basic Example

The problem is to sample from a multimodal distribution $f(x) \propto \exp\{-H(x)\}$, where

$$\begin{aligned} H(x) = &-\{x_1\sin(20x_2) + x_2\sin(20x_1)\}^2\cosh\{\sin(10x_1)x_1\} \\ &-\{x_1\cos(10x_2) - x_2\sin(10x_1)\}^2\cosh\{\cos(20x_1)x_1\} \end{aligned}$$

with domain $(x_1, x_2) \in [-1.1, 1.1]^2$. Before we start in detail, let's define an options list containing other parameters for our problem.

```
myoption = list()
myoption$partition = c(-Inf,seq(from=-8,to=0,length.out=41)) # energy partition
myoption$tau       = 1.0                                      # temperature
myoption$domain    = c(-1.1,1.1)                              # domain for sample space
myoption$vecpi     = as.vector(rep(1/41,41))                  # desired sampling distribution
myoption$niter     = 200000                                   # total number of iterations
myoption$stepsize  = 0.25                                     # s.d for random-walk proposal
```

Option 1 : R function

First, define a corresponding R function func_r that evaluates $H(x)$,

```
func_r = function(x){
x1 = x[1]; x2 = x[2];
val1 = (-(x1*sin(20*x2)+x2*sin(20*x1))^2)*cosh(sin(10*x1)*x1);
val2 = (-(x1*cos(10*x2)-x2*sin(10*x1))^2)*cosh(cos(20*x2)*x2);
return(val1+val2);
}
```

Option 2 : C++ function

Let's make a C++ function that does the same job,

```r
library(RcppXPtrUtils)
cppscript = "SEXP funcH(arma::vec x){
double x1 = x(0);
double x2 = x(1);
double val1 = (-std::pow((x1*sin(20*x2)+x2*sin(20*x1)),2))*cosh(sin(10*x1)*x1);
double val2 = (-std::pow((x1*cos(10*x2)-x2*sin(10*x1)),2))*cosh(cos(20*x2)*x2);
return Rcpp::wrap(val1+val2);
}"
func_ptr = RcppXPtrUtils::cppXPtr(cppscript,depends="RcppArmadillo") # as a pointer
```

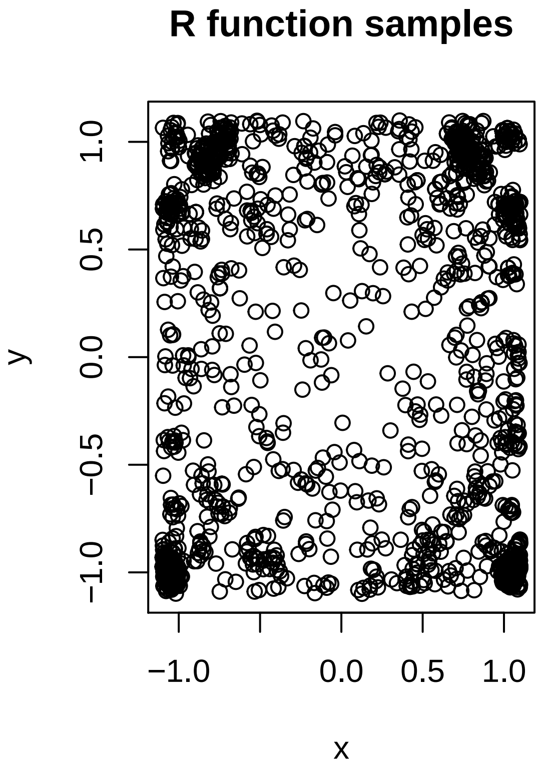
Conventional wrapping of a C/C++ chunk usually returns a wrapper that directly calls the compiled function from R. However, `cppXPtr` now returns an `XPtr` object, which is an R's traditional `externalptr` wrapped into a `XPtr` class.

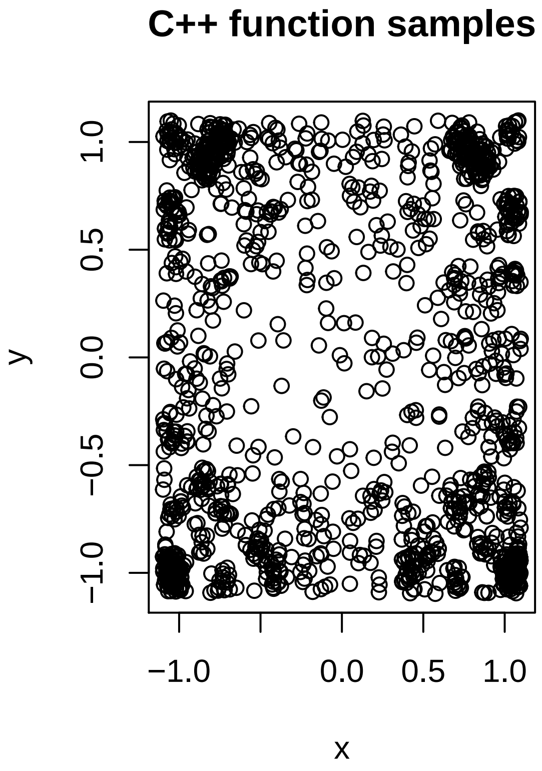
Comparison : Results

First observation should be whether two operations result in nearly identical samples.

```r
library(SAMCpack)
res1 = SAMC(2,func_r,options=myoption)        # use R function
res2 = SAMCPLUS(2,func_ptr,options=myoption) # use C++ function
```

Then, we can see that these two results are compatible,





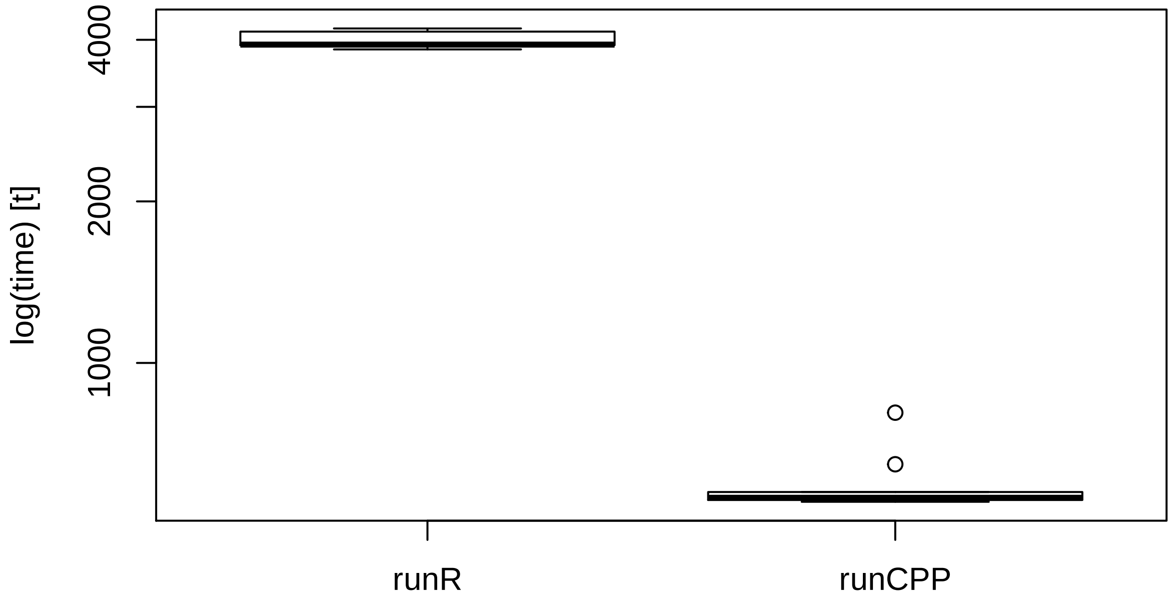
where first 100 runs are disregarded and 1/100 thinning is applied.

Comparison : Time

The most critical reason to use `SAMCPLUS` would be execution time. We ran each 10 times.

```r
library(microbenchmark)
execution = microbenchmark(
  list = alist(
    runR   = SAMC(2,func_r,options=myoption),
    runCPP = SAMCPLUS(2,func_ptr,options=myoption)
  ), times=10
)
```

and the boxplot below shows a large gap between these two methods.



How To Write a C++ Function

In the Option 2 of previous section, once a CPP script is written as an inline function, it can be wrapped as `XPtr`. In order to keep consistency across a variety code snippets and minimize potential error, we decided to impose some restrictions.

- Return type must be `SEXP`, short for S-Expression, as in `SEXP function(...)`.
- First input argument is a `arma::vec` object from RcppArmadillo, representing random variable x.
- Second input argument is used when additional data needs to be inserted through `data` argument of `SAMCPLUS`. They are should be one of
- `arma::vec` for a vector,
- `arma::mat` for a matrix, or
- R's native `List`
- When you use `List` as your data, type conversion or suitable adjustment may be required.

Why RcppArmadillo?

RcppArmadillo is a templated C++ linear algebra library. We believe it balances *ease of use* like other script computing platform and *computational efficiency*. For example, most of expressions many statisticians often use involve some degree of numerical operations and RcppArmadillo is definitely one of the optimal options if not the best. For more details about the library, please see the introductory vignette.

User-Provided Data with XPtr

As noted before, we made three options available when the compiled C++ function needs to use external data - vector(`arma::vec`), matrix(`arma::mat`), and List(`Rcpp::List`).

Case 1 : Vector/Matrix Data

We will still use the same example. First, let's consider a case to use a vector-valued data. In our example, let's call a vector $data\_vec = (10, 20)^\top$. In this case, we can define a C++ function as below.

```
data_vec = as.vector(c(10,20)) # vector-valued data=(10,20)
cppscript_vec = "SEXP funcH_vec(arma::vec x, arma::vec data){
double x1 = x(0);
double x2 = x(1);
double par1 = data(0);  // first element  : 10
double par2 = data(1);  // second element : 20
double val1 = (-std::pow((x1*sin(par2*x2)+x2*sin(par2*x1)),2))*cosh(sin(par1*x1)*x1);
double val2 = (-std::pow((x1*cos(par1*x2)-x2*sin(par1*x1)),2))*cosh(cos(par2*x2)*x2);
return Rcpp::wrap(val1+val2);
}"
```

Second, let's assume we have a matrix-valued data, say `data_mat` is

$$\begin{pmatrix} 20 & 20 & 10 \\ 10 & 10 & 20 \end{pmatrix}$$

whose elements are corresponding to the numeric values in a cost function. As before,

```
data_mat = matrix(c(20,10,20,10,10,20),nrow=2)
cppscript_mat = "SEXP funcH_mat(arma::vec x, arma::mat data){
double x1 = x(0);
double x2 = x(1);
double val1 = (-std::pow((x1*sin(data(0,0)*x2)
              +x2*sin(data(0,1)*x1)),2))*cosh(sin(data(0,2)*x1)*x1);
double val2 = (-std::pow((x1*cos(data(1,0)*x2)
              -x2*sin(data(1,1)*x1)),2))*cosh(cos(data(1,2)*x2)*x2);
return Rcpp::wrap(val1+val2);
}"
```

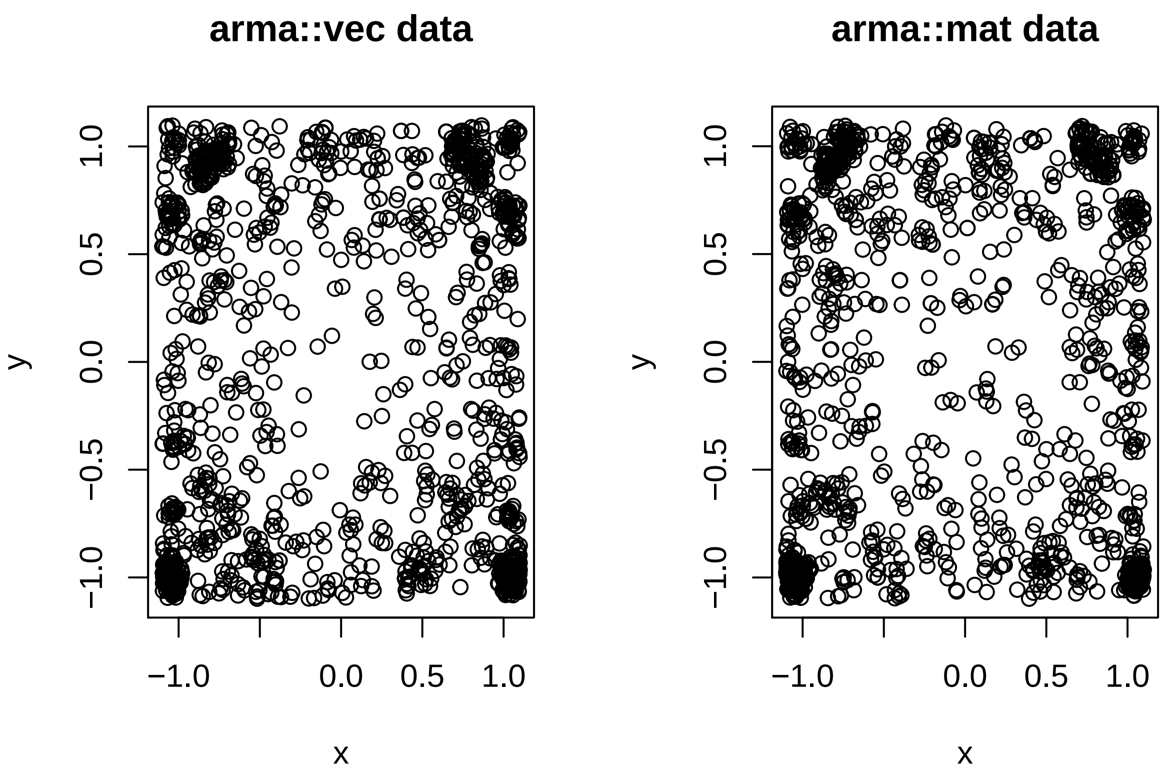
Then, create two `XPtr`'s from our supplied functions,

```
func_ptrvec = RcppXPtrUtils::cppXPtr(cppscript_vec,depends="RcppArmadillo") # as a pointer
func_ptrmat = RcppXPtrUtils::cppXPtr(cppscript_mat,depends="RcppArmadillo") # as a pointer
```

and these can be run likewise.

```
res3 = SAMCPLUS(2,func_ptrvec,options=myoption,data=data_vec) # vector data
res4 = SAMCPLUS(2,func_ptrmat,options=myoption,data=data_mat) # matrix data
```

and still we can check that the results are compatible.



Case 2 : List Data

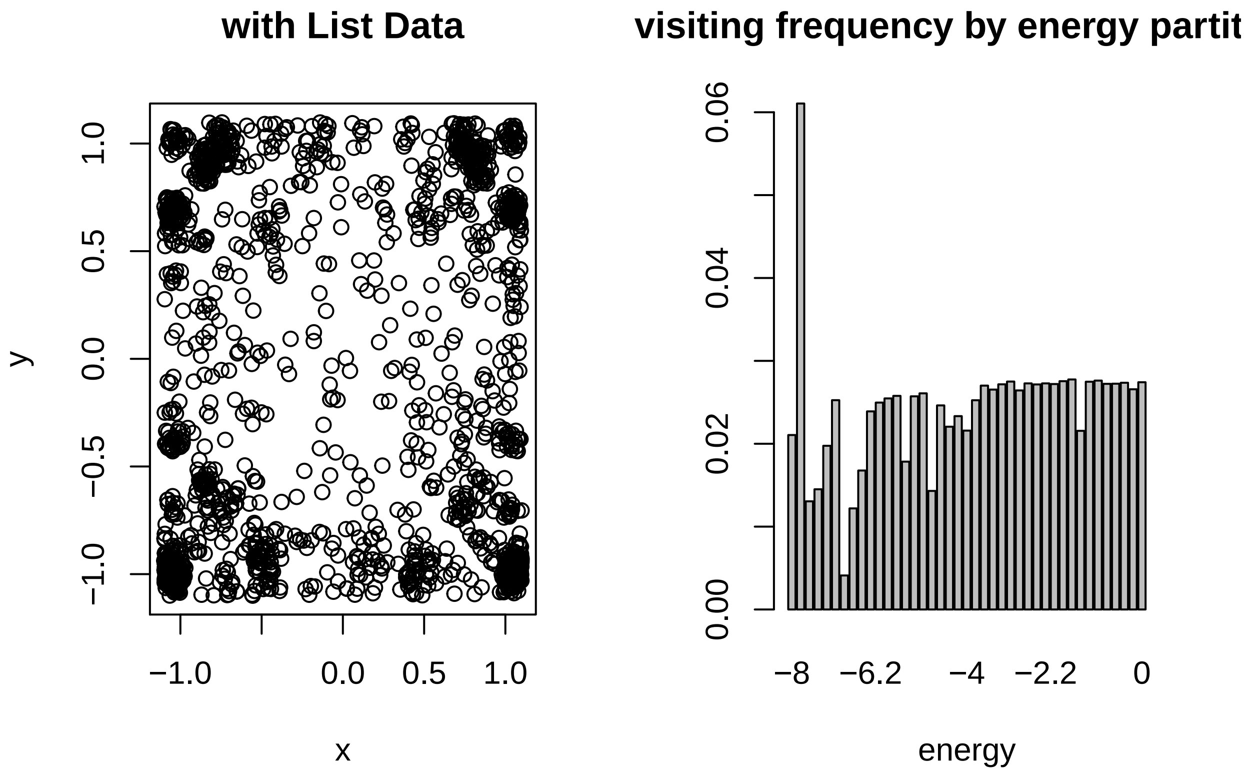
Unlike `arma::vec` and `arma::mat`, `List` is a native R and Rcpp object. List may contain multiple elements and for this scenario we will use both vector and matrix data, each. Especially, in this case, we will show how you can use `Rcpp` native vector and matrix class as well. First, let's prepare the data.

```
data_list = list()
data_list[[1]] = as.vector(c(20,10))
data_list[[2]] = matrix(c(20,10,10,20),nrow=2)
```

In the code below, vector and matrix are sequentially extracted using integer index for a list.

```
cppscript_list = "SEXP funcH_list(arma::vec x, Rcpp::List datalist){
double x1 = x(0);
double x2 = x(1);

NumericVector lefty = as<NumericVector>(datalist[0]);
NumericMatrix right = as<NumericMatrix>(datalist[1]);

double val1 = (-std::pow((x1*sin(lefty[0]*x2)
              +x2*sin(right(0,0)*x1)),2))*cosh(sin(right(0,1)*x1)*x1);
double val2 = (-std::pow((x1*cos(lefty[1]*x2)
               -x2*sin(right(1,0)*x1)),2))*cosh(cos(right(1,1)*x2)*x2);
return Rcpp::wrap(val1+val2);
}"
```

If we compile as before and run it, we can check the following results,



Case 3 : Arbitrary-Type Data

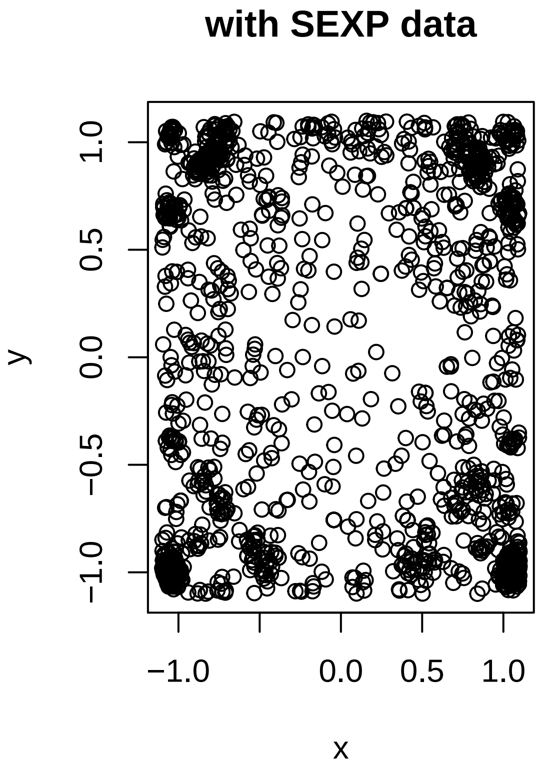
As well known, types of data available in R are indeed just SEXPs, or S-expression. Therefore, for the advanced user, we made SEXP option to be taken care of at the interface level. Below should be a replicate of using vector-type data similar to Case 1, but additional care of type conversion is required.

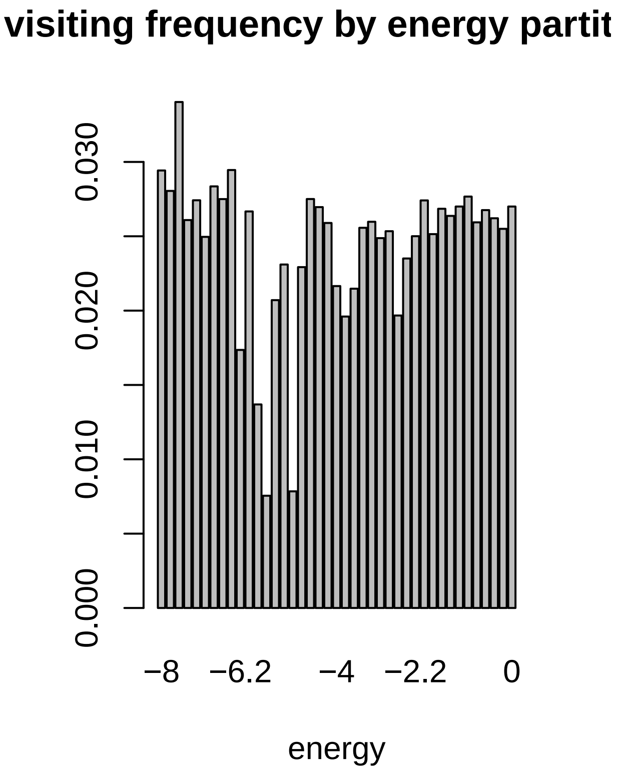
```
cppscript_sexp = "SEXP funcH_sexp(arma::vec x, SEXP data){
double x1 = x(0);
double x2 = x(1);

// Wrap the input 'data' as 'datavec' (Rcpp type)
NumericVector datavec = as<NumericVector>(data);

double par1 = datavec[0];  // first element  : 10
double par2 = datavec[1];  // second element : 20
double val1 = (-std::pow((x1*sin(par2*x2)+x2*sin(par2*x1)),2))*cosh(sin(par1*x1)*x1);
double val2 = (-std::pow((x1*cos(par1*x2)-x2*sin(par1*x1)),2))*cosh(cos(par2*x2)*x2);
return Rcpp::wrap(val1+val2);
}"
```

Let's see it ran well,

```
data_sexp = as.vector(c(10,20)) # vector-valued data=(10,20) to be passed as SEXP
func_ptrsexp = cppXPtr(cppscript_sexp,depends="RcppArmadillo")
res6 = SAMCPLUS(2,func_ptrsexp,options=myoption,data=data_sexp)
```

and the visual inspection also guarantees that it worked well.


with SEXP data
y
1.0
0.5
0.0
−0.5
−1.0
−1.0
0.0
0.5
1.0
x


visiting frequency by energy partit
0.030
0.020
0.010
0.000
−8
−6.2
−4
−2.2
0
energy