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// file: autocorrelation_test.cpp
//
// C++ Program to demonstrate the use of an autocorrelation function.
//
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//
// Revision history:
// 05/15/04 original version, based on discussion in Pang
// 02/25/05 modified comments
// 02/20/06 switched sqr to inline function
//
// Notes:
// * Compile and link with:
//   g++ -Wall -o autocorrelation_test autocorrelation_test.cpp
//   -lgsl -lgslcblas
// * gsl routines have built-in
//   extern "C" {
//     <header stuff>
//   }
//   so they can be called from C++ programs without modification
//
//*****//
// include files
#include <iostream>
#include <iomanip>
#include <fstream>
#include <cmath>
using namespace std;

#include <gsl/gsl_rng.h> // gsl random number generators
#include <gsl/gsl_randist.h> // gsl random distributions

// function prototypes
double full_integrand (double x);
double weight_function (double x);
double remaining_integrand (double x);

inline double sqr (double x) { return x*x; }; // square a double
extern unsigned long int random_seed (); // routine to generate a seed

// global variables
double lower_limit = 0.;
double upper_limit = 10.;
double norm = 1./0.886227; // norm for these integration limits

//*****
int
main (void)
{
    // width of the integral
    double volume = upper_limit - lower_limit;

    // Use the GSL random number generators (rng's)
    gsl_rng *rng_ptr = gsl_rng_alloc (gsl_rng_taus); // allocate an rng
    gsl_rng_set (rng_ptr, random_seed ()); // seed the rng
    double random = 0.; // this will be our random variable from 0 to 1

    int iterations = 10000; // Monte Carlo iterations

    // first estimate the integral based on random samples
    double sum_random = 0.; // accumulate the sum for the integral
    double sum_sq_random = 0.; // accumulate the squares for the variance
    for (int i = 0; i < iterations; i++)
    {
        random = gsl_rng_flat (rng_ptr, 0., 1.);
        double x = lower_limit + random * (upper_limit - lower_limit);
        double result = full_integrand (x);
        sum_random += result;

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        sum_sq_random += sqr (result);
    }

    double estimate_random = volume * sum_random / double(iterations);
    double error_random = volume * sqrt( (sum_sq_random/double(iterations)
                                         - sqr(sum_random/double(iterations)))
                                         /double(iterations) );

    cout << "estimate from random sampling = " << estimate_random
          << "+/- " << error_random;

    // -----
    //
    // now estimate the integral based on Metropolis
    //
    double max_step = 0.1; // maximum absolute change in x
    int initial_skip = 0; // how many initial configurations to throw away
    int skip = 1; // how often to accumulate a configuration
    double sum_metropolis = 0.; // sum for the integral
    double sum_sq_metropolis = 0.; // sum for the variance
    int successes = 0;

    // Initial configuration
    random = gsl_rng_flat (rng_ptr, 0., 1.);
    double x = lower_limit + random * (upper_limit - lower_limit);
    double weight_x = weight_function (x);

    // Loop through many Monte Carlo steps (MCS); each is just a (possible) new x
    for (int i = 0; i < initial_skip + iterations*skip; i++)
    {
        // Choose dx randomly distributed in -max_step < dx < max_step
        random = gsl_rng_flat (rng_ptr, 0., 1.);
        double dx = (2. * random - 1.) * max_step;

        double x_new = x + dx;
        if ((x_new < lower_limit) || (x_new > upper_limit))
        {
            // reject because outside of limits --> leave x unchanged
        }
        else
        {
            double weight_x_new = weight_function (x_new);
            random = gsl_rng_flat (rng_ptr, 0., 1.);
            if ( weight_x_new > (weight_x * random) )
            {
                // accept the move
                weight_x = weight_x_new;
                x = x_new;
                successes++;
            }
            else
            {
                // reject from Metropolis
            }
        }

        // accumulate the result every skip MCS
        if ((i >= initial_skip) && (i % skip == 0))
        {
            double result = remaining_integrand (x);
            sum_metropolis += result;
            sum_sq_metropolis += sqr (result);
        }
    }

    double estimate_metropolis = sum_metropolis / double(iterations);
    double error_metropolis = sqrt(fabs(sum_sq_metropolis/double(iterations)
                                       - sqr(estimate_metropolis)/double(iterations)));

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cout << endl;
cout << " estimate from metropolis= " << estimate_metropolis
    << " +/- " << error_metropolis << endl;
cout << "Metropolis acceptance rate: "
    << double(successes) / double(iterations*skip)
    << endl;

return 0;
}

//*****

double
full_integrand (double x)
{
return ( norm * sqr(x) * exp(-sqr(x)) );
}

//*****

double
weight_function (double x)
{
return ( exp(-sqr(x)) );
}

//*****

double
remaining_integrand (double x)
{
return ( sqr(x) );
}

//*****
```