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// file: derivative_test.cpp
//
// Program to study the error in differentiation rules
//
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//
// Revision history:
// 01/14/04  original version, translated from derivative_test.c
// 01/14/07  modified to be consistent with derivative_test_simple.cpp
//
// Notes:
// * Based on the discussion of differentiation in Chap. 8
//   of "Computational Physics" by Landau and Paez.
// * Use the adaptive gsl_diff_central function as well.
//   Output from this with  $e^{-x}$  at  $x=1$  is:
//   gsl_diff_central(1) = -3.6787944117560983e-01 +/- 6.208817e-04
//   actual relative error: 1.13284386e-11
//*****
// include files
#include <iostream>           // note that .h is omitted
#include <iomanip>            // note that .h is omitted
#include <fstream>           // note that .h is omitted
using namespace std;       // we need this when .h is omitted
#include <gsl/gsl_math.h>
#include <gsl/gsl_diff.h>

// function prototypes
double test_function (double x, void *params_ptr);
double test_function_derivative (double x, void *params_ptr);

double forward_diff (double x, double h,
                    double (*f) (double x, void *params_ptr),
                    void *params_ptr);
double central_diff (double x, double h,
                    double (*f) (double x, void *params_ptr),
                    void *params_ptr);
double extrapol_diff (double x, double h,
                    double (*f) (double x, void *params_ptr),
                    void *params_ptr);

//***** main program *****
int
main (void)
{
    void *params_ptr;           // void pointer passed to functions

    const double hmin = 1.e-10; // minimum mesh size
    double x = 1.;             // find the derivative at x
    double alpha = 1.;         // a parameter for the function
    double diff_cd, diff_fd;    // central, forward difference
    double diff_extrap;        // extrapolated derivative
    double diff_gsl_cd;        // gsl adaptive central derivative
    gsl_function My_F;         // gsl function type
    double abserr;            // absolute error

    ofstream out ("derivative_test.dat"); // open the output file
    params_ptr = &alpha;      // double to pass to function

    // exact answer for test
    double answer = test_function_derivative (x, params_ptr);

    My_F.function = &test_function; // set up the gsl function
    My_F.params = params_ptr;
    gsl_diff_central (&My_F, x, &diff_gsl_cd, &abserr); // gsl calculation

    cout << "gsl_diff_central(" << x << ")=" << scientific
         << setprecision (16) << diff_gsl_cd << " +/- "

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    << setprecision (6) << abserr << endl;
    cout << " actual relative error: " << setprecision (8)
         << fabs((diff_gsl_cd - answer)/answer) << endl;

    double h = 0.1;           // initialize mesh spacing
    while (h >= hmin)
    {
        diff_fd = forward_diff (x, h, &test_function, params_ptr);
        diff_cd = central_diff (x, h, &test_function, params_ptr);
        diff_extrap = extrapol_diff (x, h, &test_function, params_ptr);

        // print relative errors to output file
        out << scientific << setprecision (8)
            << log10 (h) << " "
            << log10 (fabs ((diff_fd - answer) / answer)) << " "
            << log10 (fabs ((diff_cd - answer) / answer)) << " "
            << log10 (fabs ((diff_extrap - answer) / answer)) << endl;

        h /= 2.;              // reduce mesh by 2
    }

    out.close ();            // close the output stream
    return (0);              // successful completion
}

//***** funct *****
double
test_function (double x, void *params_ptr)
{
    double alpha;
    alpha = *(double *) params_ptr;

    return (exp (-alpha * x));
}

//***** funct_deriv *****
double
test_function_derivative (double x, void *params_ptr)
{
    double alpha = *(double *) params_ptr;

    return (-alpha * exp (-alpha * x));
}

//***** forward_diff *****
double
forward_diff (double x, double h,
             double (*f) (double x, void *params_ptr), void *params_ptr)
{
    return ( f(x + h, params_ptr) - f(x, params_ptr) ) / h;
}

//***** central_diff *****
double
central_diff (double x, double h,
             double (*f) (double x, void *params_ptr), void *params_ptr)
{
    return ( f(x + h/2., params_ptr) - f(x - h/2., params_ptr) ) / h;
}

//***** extrapol_diff *****
double
extrapol_diff (double x, double h,
              double (*f) (double x, void *params_ptr), void *params_ptr)
{
    return ( 8.*(f(x + h/4., params_ptr) - f(x - h/4., params_ptr))
           - (f(x + h/2., params_ptr) - f(x - h/2., params_ptr)) )
           / (3.*h);
}

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