EPFL

Numerical Analysis and Computational Mathematics

Fall Semester 2024 – CSE Section

Prof. Laura Grigori

Assistant: Israa Fakih

Session 7 – October 30, 2024

Numerical differentiation and integration

Exercise I (MATLAB)

Consider a function $f : [a, b] \to \mathbb{R}$ such that $f \in C^1([a, b])$. We are interested in approximating $f'(\overline{x})$ with $\overline{x} \in [a, b]$.

a) Write the MATLAB functions {forward,backward,centered}_finite_difference.m that approximate $f'(\overline{x}_j)$ at the nodes $\{\overline{x}_j\}_{j=0}^n \subset [a, b]$ for some $n \geq 0$, by means of the forward, backward, and centered finite differences, respectively.
You can start from the template forward_finite_difference_template.m.

```
function [ dfh ] = forward_finite_difference( fun, xnodes, h )
% FORWARD_FINITE_DIFFERENCE approximate the first derivative of a function
% in the nodes by using the forward finite difference scheme
%
%  [ dfh ] = forward_finite_difference( fun, xnodes, h )
%  Inputs: fun = function handle,
%          xnodes = vector of nodes' coordinates
%          h = coordinates increment; positive and scalar value.
%  Output: dfh = approximate values of the first derivatives of fun in the
%          nodes.
%
...
return
```

b) For $f(x) = x\,\log(x) - (\sin(x))^2$, approximate $f'(\overline{x})$ at $\overline{x} = 1.9$ by using the MATLAB functions implementing the forward, backward, and centered finite difference schemes from point a), thus obtaining the approximate first derivatives $(\delta_+ f)(\overline{x})$, $(\delta_- f)(\overline{x})$, and $(\delta_c f)(\overline{x})$, respectively. Take as increment $h = 1/16$, and compare the approximate derivatives with the exact value $f'(\overline{x})$.

c) Repeat point b) with $h = 2^{-k}$ for $k = 2, \dots, 7$, computing the errors

$$(e_+ f)(\overline{x}) := \left| f'(\overline{x}) - (\delta_+ f)(\overline{x}) \right|,$$

$$(e_- f)(\overline{x}) := \left| f'(\overline{x}) - (\delta_- f)(\overline{x}) \right|,$$
$$(e_c f)(\overline{x}) := \left| f'(\overline{x}) - (\delta_c f)(\overline{x}) \right|.$$

Plot the errors vs. h. What are the convergence orders of the errors? Are these in agreement with the theoretical ones? Motivate the answer.

d) We want to approximate the first derivative of the function $f(x)$ given at point b) at the nodes $x_j = a + jh$, for $j = 0, \ldots, n$, with $h = (b-a)/n$, $a = 3/2$ and $b = 5/2$. To this aim, use the centered finite difference method at all nodes in the open interval (a, b). For the extremal nodes $\overline{x}_0 = a$ and $\overline{x}_n = b$, approximate the first derivatives as $(\delta_c^+ f)(\overline{x}_0) = \left[-3f(\overline{x}_0) + 4f(\overline{x}_1) - f(\overline{x}_2)\right]/(2h)$ and $(\delta_c^- f)(\overline{x}_n) = \left[3f(\overline{x}_n) - 4f(\overline{x}_{n-1}) + f(\overline{x}_{n-2})\right]/(2h)$, respectively. Set $n = 8$ and compare the approximate derivatives at the nodes with the exact ones. Then, repeat for $n = 16$.

Exercise II (MATLAB)

Consider a function $f : [a, b] \to \mathbb{R}$ such that $f \in C^0([a, b])$; we are interested in approximating the integral $I(f) = \int_a^b f(x)\,dx$.

a) Write the MATLAB functions {`midpoint`,`trapezoidal`,`simpson`}`_composite_quadrature.m` that implement the approximation of $I(f)$ by means of the composite midpoint, trapezoidal, and Simpson quadrature formulas, respectively. You may use the template `midpoint_composite_quadrature_template.m`.

```
function [ Ih ] = midpoint_composite_quadrature( fun, a, b, M )
% MIDPOINT_COMPOSITE_QUADRATURE approximate the integral of a function in
% the interval [a,b] by means of the composite midpoint quadrature formula
%  [ Ih ] = midpoint_composite_quadrature( fun, a, b, M )
%  Inputs: fun = function handle,
%          a,b = extrema of the interval [a,b]
%          M = number of subintervals of [a,b] of the same size, M≥1
%              (the case M=1 corresponds to the simple formula)
%  Output: Ih = approximate value of the integral
%
...
return
```

b) Consider the function $f(x) = \sin(7/2\,x) + e^x - 1$, with $a = 0$ and $b = 1$. We have $I(f) = 2/7\,(1 - \cos(7/2)) + e - 2$. Use the MATLAB functions implemented at point a) to approximate the integral $I(f)$, in the *simple* case (i.e. using a single sub-interval, $M = 1$). Compare the approximate values with $I(f)$.

c) Repeat point b) by using the composite midpoint, trapezoidal, and Simpson quadrature formulas over $M = 10$ uniform sub-intervals, thus obtaining the approximated values of the integral $I^c_{mp}(f)$, $I^c_t(f)$, and $I^c_s(f)$, respectively.

d) Repeat point c) with $M = 2^k$, for $k = 2, \ldots, 7$, computing the errors

$$E^c_{mp}(f) := \left| I(f) - I^c_{mp}(f) \right|,$$

$$E^c_t(f) := \left| I(f) - I^c_t(f) \right|,$$

$$E_s^c(f) := |I(f) - I_s^c(f)|\,.$$

Plot the errors vs. $H = (b-a)/M$. What are the convergence orders? Are these in agreement with the theoretical ones (the orders of accuracy of the quadrature formulas)? Motivate the answer.

e) Set $f(x) = x^d$, $a = 0$, and $b = 1$, with $d \in \mathbb{N}$. We have $I(f) = 1/(d+1)$. By using the MATLAB functions implemented at point a), verify the degree of exactness of the midpoint, trapezoidal, and Simpson quadrature formulas by approximating the integral $I(f)$ for different values of $d = 0, 1, 2, \ldots$. Motivate the results obtained.

Exercise III (Theoretical)

Consider the functions $f_1,\ f_2 : [a,b] \to \mathbb{R}$, with $f_1(x) = 4x^2 - x - 1$, $f_2(x) = e^x - x + 1$, for $a = 0$ and $b = 1$. We are interested in approximating the integrals $I(f_i) = \int_a^b f_i(x)\,dx$ for $i = 1, 2$.

a) Calculate the errors associated to the approximation of $I(f_1)$ by means of the simple midpoint, trapezoidal, and Simpson quadrature formulas.

b) Now we turn to composite schemes, by dividing the interval $[a,b]$ uniformly into sub-intervals. Estimate the minimum number M_{min} of sub-intervals that ensures that the errors corresponding to the approximation of the integrals $I(f_i)$, with $i = 1, 2$, are smaller than $tol = 10^{-5}$. Perform the calculation for composite midpoint, trapezoidal, and Simpson quadrature formulas.

Exercise IV (Theoretical)

Given a function $f \in C^2([a,b])$, prove that the error $e_t(f)$ associated to the *simple trapezoidal quadrature formula* satisfies

$$e_t(f) := I(f) - I_t(f) = -\frac{(b-a)^3}{12} f''(\xi)$$

for some $\xi \in [a,b]$. (*Hint*: first, express the difference between f and its linear approximation over $[a,b]$ in a more manageable form, involving the nodal polynomial $(x-a)(x-b)$.)