Numerical Analysis and Computational Mathematics

Fall Semester 2019 - Section CSE

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Numerical Derivation and Integration

Exercise I (MATLAB)

Let us consider a function $f : [a, b] \to \mathbb{R}$ such that $f \in C^1([a, b])$ of which we are interested in approximating $f'(\overline{x})$ with $\overline{x} \in [a, b]$.

a) Write the MATLAB functions `forward_finite_difference.m`, `backward_finite_difference.m`, and `centered_finite_difference.m` that approximate $f'(\overline{x}_j)$ in the nodes $\{\overline{x}_j\}_{j=0}^n \in [a, b]$ for some $n \geq 0$, by means of the forward, backward, and centered finite differences, respectively.
Use the template `forward_finite_difference_template.m` as example.

```
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
```

The functions should return in a vector `dfh` the approximate derivatives of the function `fun` corresponding to the coordinates $\{\overline{x}_j\}_{j=0}^n$ contained in the vector `xnodes` by using the increment `h` (a positive scalar).

b) For $f(x) = x \log(x) - (\sin(x))^2$, approximate $f'(\overline{x})$ in $\overline{x} = 1.9$ by using the MATLAB functions implementing the forward, backward, and centered finite difference schemes of point a), thus obtaining the approximate first derivatives $(\delta_+ f)(\overline{x})$, $(\delta_- f)(\overline{x})$, and $(\delta_c f)(\overline{x})$, respectively. Assume 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 $k = 2, \ldots, 7$ by computing $(e_+ f)(\overline{x}) := |f'(\overline{x}) - (\delta_+ f)(\overline{x})|$, $(e_- f)(\overline{x}) := |f'(\overline{x}) - (\delta_- f)(\overline{x})|$, and $(e_c f)(\overline{x}) := |f'(\overline{x}) - (\delta_c f)(\overline{x})|$ corresponding to the errors of the forward, backward, and centered finite difference schemes, respectively. Plot the errors vs. h in logarithmic scales on both the axes. What are the convergence orders of the errors? Are these in agreement with the theoretical ones? Motivate the answer.

d) Approximate the first derivatives of the function $f(x)$ given at point b) in the nodes $x_j \in [a, b]$ for $j = 0, \ldots, n$, with $h = (b - a)/n$; we set $a = 3/2$ and $b = 5/2$. With this aim, consider the centered finite difference method implemented in the MATLAB function at point a) for the approximation of $f'(\overline{x}_j)$ in the nodes internal the interval $[a, b]$, i.e. in $\overline{x}_j \in (a, b)$ with $j = 1, \ldots, n-1$. For the extrema nodes $\overline{x}_0 = a$ and $\overline{x}_n = b$ approximate the first derivatives as $\widetilde{(\delta_c f)}(\overline{x}_0) = \left[-3f(\overline{x}_0) + 4f(\overline{x}_1) - f(\overline{x}_2)\right]/(2h)$ and $\widetilde{(\delta_c f)}(\overline{x}_n) = \left[3f(\overline{x}_n) - 4f(\overline{x}_{n-1}) + f(\overline{x}_{n-2})\right]/(2h)$, respectively. Set $n = 8$ and compare the approximate derivatives in the nodes with the exact ones; then, repeat for $n = 16$.

Exercise II (MATLAB)

Let us 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_composite_quadrature.m`, `trapezoidal_composite_quadrature.m`, and `simpson_composite_quadrature.m` that implement the approximation of $I(f)$ by means of the composite midpoint, trapezoidal, and Simpson quadrature formulas, respectively.
Use the template `midpoint_composite_quadrature_template.m` as example.

```
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
```

The inputs of the functions are: `fun` (the function handle of $f(x)$), the extrema of the interval `a`, `b`, and `M`, the number of subintervals of the same size M in which $[a, b]$ is subdivided.

b) Let us consider the function $f(x) = \sin(7/2\, x) + e^x - 1$ with $a = 0$ and $b = 1$ ($f \in C^\infty([a, b])$) for which $I(f) = 2/7\,(1 - \cos(7/2)) + e - 2$. Use the the MATLAB functions implemented at point a) to approximate the integral $I(f)$ by means of the *simple midpoint, trapezoidal*, and *Simpson quadrature formulas*. Report the values of the approximated integrals in comparison with $I(f)$.

c) Repeat point b) by using the *composite midpoint, trapezoidal*, and *Simpson quadrature formulas* with $M = 10$ subintervals of the same size, 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 $k = 2, \ldots, 7$ by computing the errors $E^c_{mp}(f) := \left|I(f) - I^c_{mp}(f)\right|$, $E^c_t(f) := |I(f) - I^c_t(f)|$, and $E^c_s(f) := |I(f) - I^c_s(f)|$ corresponding to the composite midpoint, trapezoidal, and Simpson quadrature formulas, respectively. Plot the errors vs. $H = (b-a)/M$ in logarithmic scales on both the axes. What are the convergence orders of the errors (orders of accuracy of the quadrature formulas)? Are these in agreement with the theoretical ones? Motivate the answer.

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

Exercise III (Theoretical)
Let us consider the functions $f_1,\ f_2 : [a, b] \to \mathbb{R}$, with $f_1(x) = 4x^2 - x - 1$, $f_2(x) = e^x - x + 1$, $a = 0$, and $b = 1$, for which $f_1,\ f_2 \in C^\infty([a, b])$. 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 $I(f_1)$, the integral of the function $f_1(x)$, by means of the *simple midpoint, trapezoidal*, and *Simpson quadrature formulas.*

b) Estimate the minimum number of subintervals of the same size which subdivide the interval $[a, b]$, say M_{min}, ensuring that the errors corresponding to the approximation of the integrals $I(f_i)$, with $i = 1, 2$, by means of the *composite midpoint, trapezoidal*, and *Simpson quadrature formulas* are inferior to the tolerance $tol = 10^{-5}$. Motivate the results obtained.

Exercise IV (Theoretical)
Let us consider a function $f \in C^2([a, b])$, prove that the error $e_t(f)$ associated to the *simple trapezoidal quadrature formula* reads:

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

for some $\xi \in [a, b]$.