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MATH 174 – B2L

Exercise 4.1: Numerical Differentiation

We wish to derive a four-point backward formula of order three which approximates the derivative of a function $f(x)$ at a number x, i.e., approximate the quantity $f'(x)$. Suppose we let a uniform increment $h > 0$ for our four arbitrary data points. With this, we construct a formula that needs $f(x), f(x-h), f(x-2h)$ and $f(x-3h)$ in our derivation.

By Taylor's theorem, the expansion for $f(x-h), f(x-2h)$ and $f(x-3h)$ are given as follows:

$$\begin{cases} f(x-h) = f(x) - hf'(x) + \frac{h^2 f''(x)}{2!} - \frac{h^3 f'''(x)}{3!} + \frac{h^4 f^{(4)}(x)}{4!} + \dots \\ f(x-2h) = f(x) - 2hf'(x) + \frac{4h^2 f''(x)}{2!} - \frac{8h^3 f'''(x)}{3!} + \frac{16h^4 f^{(4)}(x)}{4!} + \dots \\ f(x-3h) = f(x) - 3hf'(x) + \frac{9h^2 f''(x)}{2!} - \frac{27h^3 f'''(x)}{3!} + \frac{81h^4 f^{(4)}(x)}{4!} + \dots \end{cases} \tag{1}$$

Note that f'' and f''' are unknowns and we restrict ourselves to have no formula or procedure to find their expressions. Hence, we want to eliminate the terms of the expressions in (1) with f'' and f''' by finding multipliers $A, B,$ and C to $f(x-h), f(x-2h)$ and $f(x-3h)$, respectively, such that

$$Af(x-h) + Bf(x-2h) + Cf(x-3h) \tag{2}$$

will have no terms with f'' and f'''. From (2) applied to (1), we obtain the linear system below:

$$\begin{cases} A + 4B + 9C = 0 \\ -A - 8B - 27C = 0 \end{cases} \implies \begin{cases} A + 4B + 9C = 0 \\ A + 8B + 27C = 0 \end{cases}$$

Observe that there are 2 linear equations with 3 unknowns. Hence, it is expected that the solution set to the system is an infinite collection of triples. By elimination and substitution method, we obtain that

$$C = \frac{1}{9}A$$

and

$$B = \frac{-9}{2}C = \frac{-9}{2}\left(\frac{1}{9}A\right) = \frac{-1}{2}A$$

And so, the solution set to the system is

$$\left\{ \left(A, \frac{-1}{2}A, \frac{1}{9}A \right) \mid A \in \mathbb{R} \right\}$$

Suppose we take $A = 1$, then $B = -\frac{1}{2}$ and $C = \frac{1}{9}$. Substituting these to equation (2) and using the expansions from (1), we have

$$\begin{aligned} f(x-h) - \frac{1}{2}f(x-2h) + \frac{1}{9}f(x-3h) &= \left(1 - \frac{1}{2} + \frac{1}{9}\right) f(x) - \left(1 - \frac{2}{2} + \frac{3}{9}\right) hf'(x) + \left(1 - \frac{16}{2} + \frac{81}{9}\right) \frac{h^4 f^{(4)}(x)}{4!} + \dots \\ &= \frac{11}{18} f(x) - \frac{1}{3} hf'(x) + 2\frac{h^4 f^{(4)}(x)}{4!} + \dots \end{aligned}$$

Notice that the terms with f' and f'' cancels out so we obtain the simplified equation above. Simplifying this equation further and isolating $f'(x)$, we have

$$\begin{aligned} \frac{1}{3}hf'(x) &= \frac{11}{18}f(x) - f(x-h) + \frac{1}{2}f(x-2h) - \frac{1}{9}f(x-3h) + \frac{h^4 f^{(4)}(x)}{12} + \dots \\ f'(x) &= \frac{11}{6h}f(x) - \frac{3}{h}f(x-h) + \frac{3}{2h}f(x-2h) - \frac{1}{3h}f(x-3h) + \frac{h^3 f^{(4)}(\xi)}{4} \\ &= \frac{11f(x) - 18f(x-h) + 9f(x-2h) - 2f(x-3h)}{6h} + \mathcal{O}(h^3) \end{aligned}$$

This implies that we obtain the formula

$$f'(x) \approx \frac{11f(x) - 18f(x-h) + 9f(x-2h) - 2f(x-3h)}{6h} \tag{3}$$

with theoretical error

$$\frac{h^3 f^{(4)}(\xi)}{4}$$

for some $\xi \in (x - 3h, h)$. (9 pts)

Now, we wish to apply the formula obtained to the function $f(x) = e^x$ and obtain an estimate for $f'(1) = e$. From (3), we obtain the formula below

$$f'(x) \approx \frac{11e^x - 18e^{x-h} + 9e^{x-2h} - 2e^{x-3h}}{6h} \tag{4}$$

which we will use to find an estimate for $f'(1) = e$. We shall find the values of the estimates for the following values of the increment: $h = 1, 0.1, 0.001, \dots, 10^{-20}$.

Using MATLAB, we obtain the estimates for each increment h. Moreover, the relative errors are computed using the formula

$$\text{relative error} = \frac{|\text{exact} - \text{estimate}|}{|\text{exact}|}$$

The obtained values are tabulated and are presented below.

Table 4.1. The estimates and their corresponding relative errors for each value of h from 10^0 to 10^{-20}.

(10pts)

h	Estimate (rounded to 10 significant figures)	Relative error (in %, rounded to 10 significant figures)
1	2.490224086	8.389775478×10^0
10^{-1}	2.717678423	$2.219805148 \times 10^{-2}$
10^{-2}	2.718281157	$2.470207411 \times 10^{-5}$
10^{-3}	2.718281828	$2.499155977 \times 10^{-8}$
10^{-4}	2.718281828	$2.298634055 \times 10^{-11}$
10^{-5}	2.718281828	$2.201248429 \times 10^{-9}$
10^{-6}	2.718281829	$7.601012655 \times 10^{-9}$
10^{-7}	2.718281814	$5.151871001 \times 10^{-7}$
10^{-8}	2.718281837	$3.016693353 \times 10^{-7}$
10^{-9}	2.718280416	$5.197714358 \times 10^{-5}$
10^{-10}	2.718280416	$5.197714358 \times 10^{-5}$
10^{-11}	2.718270053	$4.331768211 \times 10^{-4}$
10^{-12}	2.718714143	$1.590395221 \times 10^{-2}$
10^{-13}	2.716345667	$7.122740264 \times 10^{-2}$
10^{-14}	2.634929312	3.066367726×10^0
10^{-15}	3.108624469	1.435990324×10^1
10^{-16}	-5.921189465	3.178283871×10^2
10^{-17}	14.80297366	6.445709678×10^2
10^{-18}	-148.0297366	5.545709678×10^3
10^{-19}	-1480.297366	5.455709678×10^4
10^{-20}	-14802.97366	5.446709678×10^5

(3pts)

As observed, the minimal relative error is obtained when $h = 10^{-4}$. Moreover, the relative errors of the estimates obtained are progressively decreasing but only until the value of h is 10^{-4}. In particular, the relative errors decrease by a factor of 10^3 from $h = 10^0$ to $h = 10^{-4}$. This reflects the order of theoretical error we obtained in our derivation for the formula for f' which is three.

However, it is also noted from the table that from $h = 10^{-5}$ to $h = 10^{-20}$, the relative errors are increasing by factors of at most 10^2. That is, the trend we observed from $h = 10^0$ to $h = 10^{-4}$ changes once the value of h becomes 10^{-5}. This is opposite of what we may infer that the relative errors are continuously decreasing as we decrease the value of the increments of the data points. This change in trend is inferred to be the cause of the formula we constructed for $f'(x)$.

7pts

Notice in equation (4) that the denominator is a constant multiple of h. As we make the increments h smaller, the value of $\frac{1}{h}$ approaches $+\infty$. This causes the obtained value for the estimate to become larger and thus, deviating more from the exact value $f'(1) = e$. This increasing deviation causes the relative error of the estimate to also increase.

(1pt)

Appendix A

Program Used in MATLAB to construct Table 4.1

```
% 4-point backward formula of order three
clc
clear
format long

syms x
%%  Initializing Constants and Functions
f = exp(x);  % function to approximate
a = 1;  % where f'(a) is the value to approximate
numh = 21;  % no. of increments
numPts = 4;  % no. of data points

%% Icrements h and x values

% constructing uniform increments h
h = ones(1, numh);
h = 10*h;
for i = 1:numh
    h(i) = h(i)^(1-i);
end

% constructing x's using different h
% the output is a numPts x numh matrix
% each column is a group of x's for a specific h
% the h value for each column in X is in
% the same indexed column of the h array
X = zeros(numPts, numh);
X(1,:) = a*ones(1, numh);  % entries in first row of X = a
for j = 1:numh
    for i = 2:numPts  % starts iteration on 2nd row
        X(i, j) = X(1,j) - (i-1)*(h(j));  % (x-h), (x-2h), (x-3h)
    end
end

F = exp(X);  % f(x) = e^x

%%  Calculation of f'(a) and relative error

% f'(a)
Fprime = zeros(1, numh);
for j = 1:numh
    num = 11*F(1,j) - 18*F(2,j) + 9*F(3,j) - 2*F(4,j);
    den =6*h(j);
    Fprime(j) = num/den;  % approximating formula
end
disp("f'(1) = ")
disp(Fprime)

% relative error
relError = zeros(1, numh);
exact = double(subs(f, 1));
```

```
for j = 1:numh
    numer = exact - Fprime(j);
    relError(j) = abs(numer/exact);
end

disp('relative errors (in %) =')
disp(vpa(relError*100, 6)')
```