HW 4

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1. Using Taylor series, derive the following second order accurate approximation to $f''(x)$, assuming that $f \in C^4[x-h, x+h]$:

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}. \tag{1}$$

Show that the error term is $-(h^2/12)f''''(\xi)$, for some point $\xi \in [x-h, x+h]$.

Use Matlab (or a language of your choice) to evaluate (1) for $f(x) = \sin(x)$ and $x = \pi/6$. Try $h = 10^{-1}, 10^{-2}, \ldots, 10^{-16}$, and make a table of values of h, the computed finite difference quotient, and the error (which you can compute analytically since $f''(x) = -\sin(x)$ and $\sin(\pi/6) = 1/2$). Explain your results. In particular, explain why you obtained the greatest accuracy with a particular value of h and why you get totally wrong answers for some values of h.

First note by Taylor's theorem we have:

$$f(x-h) \approx f(x) - hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f''''(\varepsilon)$$

$$f(x+h) \approx f(x) + hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f''''(\varepsilon)$$

Then add two equations we have:

$$f(x-h) + f(x+h) \approx 2f(x) + h^2 f''(x) + \frac{h^4}{12}f''''(\varepsilon)$$

$$\Rightarrow \boxed{f''(x) \approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}}$$

Then note from the upper expression we have:

error term: $-\frac{h^2}{12}f''''(\varepsilon)$ for $\varepsilon \in [x-h, x+h]$

Table:

h	Computed f''(x)	Error
0.1	-0.49958	0.00041653
0.01	-0.5	4.1667e-06
0.001	-0.5	4.1674e-08
0.0001	-0.5	3.0387e-09
1e-05	-0.5	5.9648e-07
1e-06	-0.49993	6.6572e-05
1e-07	-0.49405	0.0059508
1e-08	-1.1102	0.61022
1e-09	55.511	56.011
1e-10	0	0.5
1e-11	0	0.5
1e-12	0	0.5
1e-13	5.5511e+09	5.5511e+09
1e-14	-5.5511e+11	5.5511e+11
1e-15	0	0.5
1e-16	-5.5511e+15	5.5511e+15

First note we have the greatest accuracy when h is 10^{-4} and 10^{-3}.

Then note the calculations are no longer reliable because the limitations of floating representation.

For those that have small error provides a good balance between truncation error and round off error.

For those that are way off is due to the round off error.

11. Estimate the number of subintervals required to obtain $\int_0^1 e^{-x^2}dx$ to 6 correct decimal places (absolute error $\le \frac{1}{2}\times 10^{-6}$)

(a) by means of the composite trapezoidal rule,
(b) by means of the composite Simpson's rule.

First note we have:

$f(x)=e^{-x^2}$, $f'(x)=-2xe^{-x^2}$, $f''(x)=-2e^{-x^2}+4x^2e^{-x^2}$

$f'''(x)=4xe^{-x^2}+8xe^{-x^2}-8x^3e^{-x^2}=12xe^{-x^2}-8x^3e^{-x^2}$

$f''''(x)=12e^{-x^2}-24x^2e^{-x^2}-24x^2e^{-x^2}+16x^4e^{-x^2}$

$=12e^{-x^2}-48x^2e^{-x^2}+16x^4e^{-x^2}$

a) First note from trapezoidal rule we have:

$E_n^T(f)=-\frac{1}{12}h^2(b-a)f''(\varepsilon)$, $a<\varepsilon<b$

plug in $a=0$, $b=1$ we have:

$E_n^T(f)=-\frac{1}{12n^2}f''(\varepsilon)$, $0<\varepsilon<1$

Then we have:

$E_n^T(f)=-\frac{1}{12n^2}f''(\varepsilon)$, $0<\varepsilon<1$

Note that $f'''(x)>0$ on $[0,1]$ which means that $f''(x)$ is increasing on $[0,1]$

Then plug in 0 and 1 into $f''(x)$ we have:

$f''(0)=-2$, $f''(1)=2e^{-1}$

$\Rightarrow |f''(x)|\le 2$ for $x\in[0,1]$

Then we have:

$|E_n^T(f)|=|-\frac{1}{12n^2}f''(\varepsilon)|\le\frac{1}{6n^2}\le\frac{1}{2\cdot10^6}$

$\Rightarrow 6n^2\ge 2\cdot10^6 \Rightarrow n^2\ge\frac{1}{3}\cdot10^6\Rightarrow n\ge(\frac{1}{3})^{\frac{1}{2}}10^3\approx 578$

Thus the required subinterval is $\boxed{578}$

b) Note by Simpson's rule we have:

$E_n^S(f)=-\frac{1}{180}(b-a)h^4f''''(\varepsilon)$, $a<\varepsilon<b$

plug in $a=0$, $b=1$ we have:

$E_n^S(f)=-\frac{1}{180n^4}f''''(\varepsilon)$, $0<\varepsilon<1$

Then note $f^{(5)}(x)=-24xe^{-x^2}-96xe^{-x^2}+96x^3e^{-x^2}+64x^3e^{-x^2}-32x^5e^{-x^2}$

$=-120xe^{-x^2}+160x^3e^{-x^2}-32x^5e^{-x^2}$

$=-8xe^{-x^2}(4x^4-20x^2+15)$

Then note for $x\in[0,1]$, $f^{(5)}(x)=0$ for $x=0.9586$

Then we have $f^{(5)}(x)\ge 0$ for $0\le x\le 0.9586$

$f^{(5)}(x)\le 0$ for $0.9586\le x\le 1$.

Then we have $f^{(4)}(x)$ decreases from 12 to -7.4 and increase to -7.36

$\Rightarrow |f''''(x)|\le 12$

$\Rightarrow |E_n^S(f)|=|-\frac{1}{180n^4}f^{(4)}(\varepsilon)|\le\frac{12}{180n^4}=\frac{1}{15n^4}\le\frac{1}{2\cdot10^6}$

$\Rightarrow 15n^4\ge 2\cdot10^6$

$n^4\ge\frac{2}{15}10^6$

$n\ge\sqrt{\frac{2}{15}10^6}\approx 20$

Thus the required subinterval is $\boxed{20}$

3. Construct the 2-point weighted Gauss quadrature formula for the interval $[0,1]$ with weight function $w(x) = x$; that is, find a formula of the form

$$\int_0^1 x f(x)\, dx \approx a_0 f(x_0) + a_1 f(x_1)$$

that is exact for all polynomials of degree 3 or less.

First note Gauss quadrature has a maximum degree of exactness of $2n-1$

Since we want it to exact of all polynomials of degree 3 or less.

Set up the orthogonal polynomial we have:

$\pi_2(x) = x^2 + p_1 x + p_2$

Then note it's orthogonal to 1 and x.

We have:

$$\int_0^1 x(x^2+p_1x+p_2)dx = \frac{1}{4}x^4 + \frac{1}{3}p_1x^3 + \frac{1}{2}p_2x^2\Big|_0^1$$
$$= \frac{1}{4} + \frac{1}{3}p_1 + \frac{1}{2}p_2 = 0$$

$$\int_0^1 x^2(x^2+p_1x+p_2)dx = \frac{1}{5}x^5 + \frac{1}{4}p_1x^4 + \frac{1}{3}p_2x^3\Big|_0^1$$
$$= \frac{1}{5} + \frac{1}{4}p_1 + \frac{1}{3}p_2 = 0$$

Then we have:

$$\begin{cases} \frac{1}{3}p_1 + \frac{1}{2}p_2 = -\frac{1}{4} \\ \frac{1}{4}p_1 + \frac{1}{3}p_2 = -\frac{1}{5} \end{cases}$$

$\Rightarrow p_1 = -\frac{6}{5}, \ p_2 = \frac{3}{10}$

$\Rightarrow \pi_2(x) = x^2 - \frac{6}{5}x + \frac{3}{10}$

$\Rightarrow x_0 = \frac{6+\sqrt{6}}{10}, \ x_1 = \frac{6-\sqrt{6}}{10}$

Then we expresses the fact the formula is exact for $f(x)\equiv 1$ and $f(x)\equiv x$:

$a_0 + a_1 = \int_0^1 x\,dx = \frac{1}{2}$

$a_0x_0 + a_1x_1 = \int_0^1 x^2 dx = \frac{1}{3}$

$$\Rightarrow a_0 = \frac{\frac{1}{2}x_1 - \frac{1}{3}}{x_1 - x_0} \qquad a_1 = \frac{-\frac{1}{2}x_0 + \frac{1}{3}}{x_1 - x_0}$$

$x_1 - x_0 = -\frac{\sqrt{6}}{5}$

$$a_0 = -\frac{5}{\sqrt{6}}\left(\frac{6-\sqrt{6}}{20} - \frac{1}{3}\right) \qquad a_1 = -\frac{5}{\sqrt{6}}\left(-\frac{6+\sqrt{6}}{20} + \frac{1}{3}\right)$$
$$\approx 0.31804 \qquad\qquad \approx 0.18196$$

$$\Rightarrow \boxed{\int_0^1 x f(x)dx \approx 0.31804 f\left(\frac{6+\sqrt{6}}{10}\right) + 0.18196 f\left(\frac{6-\sqrt{6}}{10}\right)}$$

4. Write a code to compute the integral of a given function using Romberg integration and to count the number of function evaluations needed to obtain a given level of accuracy. Use it to compute

$$\int_0^1 \cos(x^2)\,dx.$$

Turn in a listing of your code. Determine (experimentally) how many function evaluations are required in order to obtain an error of size 10^{-12}. Compare this with the number of function evaluations that would be required by the composite trapezoidal rule (which you can determine analytically, as in problem 2). You may also compare your results with results from **chebfun**, which uses Clenshaw-Curtis quadrature. To do this, you can type `f = chebfun('cos(x^2)',[0,1])`, `intf = sum(f)`. The package will inform you of the length of `f`, which is 1 plus the degree of the polynomial that it has used in order to compute this integral to about the machine precision. How does this compare to the number of function evaluations that you used?

Trapezoidal rule:

$f(x) = \cos(x^2)$ $\quad f'(x) = -2x\sin(x^2)$ $\quad f''(x) = -2\sin(x^2) - 4x^2\cos(x^2)$

$f'''(x) = -12x\cos(x^2) + 8x^3\sin(x^2)$

First note from trapezoidal rule we have:

$E_n^T(f) = -\frac{1}{12}h^2(b-a)f''(\varepsilon)$, $a<\varepsilon<b$

plug in $a=0$, $b=1$ we have:

$E_n^T(f) = -\frac{1}{12n^2}f''(\varepsilon)$, $0<\varepsilon<1$

Then we have:

$E_n^T(f) = -\frac{1}{12n^2}f''(\varepsilon)$, $0<\varepsilon<1$

Note $f'''(x)=0$ at $x = 0.9941$

$\Rightarrow |f''(x)| \leq 3.845$

$\Rightarrow |E_n^T(f)| \leq \frac{1}{12n^2}3.845 \leq 10^{-12}$

$\Rightarrow 12n^2 \geqslant 3.845 \cdot 10^{12}$

$n^2 \geqslant \frac{3.845}{12}\cdot 10^{12}$ $\quad n \geqslant 566053.59$

$n = \boxed{566054}$

```
% AMATH 585 HW4 Problem 4
% Tianbo Zhang 1938501
% Implementation for Romberg Extrapolation in probolem 4

% Set up the conditions
a = 0;
b = 1;
n = 100;
tol = 1e-12;
[integral, num_eval] = rombergIntegration(a, b, n, tol);
fprintf('Integral: %.15f\n', integral);
fprintf('Number of function evaluations: %d\n', num_eval);

function [integral, num_eval] = rombergIntegration(a,b,n, tol)
% Set up the base condition
    num_eval = 2;
    T=zeros(n,n);
    h=b-a;
    T(1,1)=h*(f(a)+f(b))/2;
    m = 1;
    for i=2:n
        % Trapezoidal rule
        h=h/2;
        sum = 0;
        m = 2*m;
        mm = m-1;
        for k = (1:2:mm)
            sum = sum + f(a+k*h);
        end
        T(i,1)=T(i-1,1)/2+h*sum;

        % Romberg extrapolation
        for k=2:i
            T(i,k)=T(i,k-1)+(T(i,k-1)-T(i-1,k-1))/(4^(k-1)-1);
        end

        % Check for tolerance
        num_eval = num_eval + 2^(i-2);
        integral = T(i,i);
        if abs(T(i,i) - T(i-1, i-1)) < tol
            return;
        end
    end
end

% Function to integrate
function y = f(x)
    y = cos(x.^2);
end
```

Results:

Romberg Integration:

```
>> AMATH585_hw4_p4
Integral: 0.904524237900272
Number of function evaluations: 65
```

Clenshaw - Curtis Quadrature:

```
f =

   chebfun column (1 smooth piece)
       interval       length     endpoint values
[       0,        1]       19          1     0.54
vertical scale =   1


intf =

    0.9045
```

Romberg vs. Trapezoidal:

The function of evaluation is much smaller than composite trapezoidal.

Romberg vs. Clencaw:

Clensaw requires less function evaluations than Romberg.