Part II Determine Error Bounds

Task

1. Review Simpson's Rule

Simpson's Rule is a method to numerically integrate a function where the function is approximated using parabolas. The formula for implementing Simpson's Rule is

$$\int_a^b f(x)\,dx \approx S_n = \frac{\Delta x}{3}\left[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\cdots+2f(x_{n-2})+4f(x_{n-1})+f(x_n)\right]$$

where n is the number of intervals and $\Delta x = \dfrac{b-a}{n}$. [4]

Note: n must be an even number.

2. Find Error Bound

The error bound E_S for Simpson's Rule is given by

$$|E_S| \le \frac{K(b-a)^5}{180n^4},$$

where $\left|f^{(4)}(x)\right| \le K$ for $a \le x \le b$ and $f^{(4)}(x)$ is the 4th derivative of $f(x)$. [4]

a) Find the 4th derivative of e^{-x^2} and then find the maximum value of the 4th derivative over the limits of integration.

$$f(x) = e^{-x^2}$$

$$f' = -2xe^{-x^2}$$

$$f'' = -2e^{-x^2} + 4x^2e^{-x^2} \Rightarrow f'' = e^{-x^2}\left(4x^2-2\right)$$

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

$$f^{(4)} = -2xe^{-x^2}\left(-8x^3+12x\right) + e^{-x^2}\left(-24x^2+12\right)$$

$$f^{(4)} = e^{-x^2}\left(16x^4-48x^2+12\right)$$

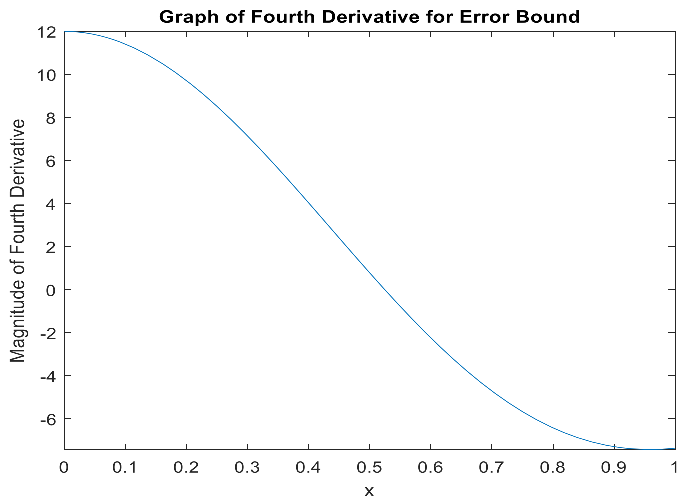

Figure 3: Graph of fourth derivative of e^{-x^2}.

At $x=0,\ f^{(4)}=12,$ at $x=1,\ f^{(4)}\approx -7.4$

$\left|f^{(4)}\right|\le 12$ for $0\le x\le 1$

b) Find n so that $E_S < 0.0001$.

$$|E_S| \le \frac{K(b-a)^5}{180n^4},$$

$$0.0001=\frac{12(1-0)^5}{180n^4} \Rightarrow n^4=\frac{12}{180(0.0001)}$$

$$n=\sqrt[4]{666.667}\approx 5$$

Need $n=6$

3. Review Taylor Polynomials

The Taylor series of a function $f(x)$ that has a power series expansion at a, is of the form

$$f(x)=\sum_{n=0}^{\infty}\frac{f^{(n)}(a)}{n!}(x-a)^n$$

$$= f(a)+\frac{f'(a)}{1!}(x-a)+\frac{f''(a)}{2!}(x-a)^2+\frac{f'''(a)}{3!}(x-a)^3+\cdots$$

a) Find the Taylor polynomial for $f(x)=e^{-x^2}$ at $a=0$.

Since

$$e^{x}=1+x+\frac{x^2}{2!}+\frac{x^3}{3!}+\frac{x^4}{4!}+\ldots=\sum_{n=0}^{\infty}\frac{x^n}{n!},$$

that gives

$$e^{-x^2}=1-x^2+\frac{x^4}{2!}-\frac{x^6}{3!}+\cdots+(-1)^n\frac{x^{2n}}{n!}=\sum_{n=0}^{\infty}(-1)^n\frac{x^{2n}}{n!}\quad .$$

b) Integrate the Taylor polynomial

Integrating the polynomial gives

$$\int e^{-x^2}dx=x-\frac{x^3}{3}+\frac{x^5}{5\cdot 2!}-\frac{x^7}{7\cdot 3!}+\frac{x^9}{9\cdot 4!}-\frac{x^{11}}{11\cdot 5!}+\frac{x^{13}}{13\cdot 6!}-\frac{x^{15}}{15\cdot 7!}+\cdots+C$$

$$=x-\frac{x^3}{3}+\frac{x^5}{10}-\frac{x^7}{42}+\frac{x^9}{216}-\frac{x^{11}}{1320}+\frac{x^{13}}{9360}-\frac{x^{15}}{75600}+\cdots+C$$

Evaluating the integral at the limits of integration, gives

$$\int_0^1 e^{-x^2}dx=1-\frac{1}{3}+\frac{1}{10}-\frac{1}{42}+\frac{1}{216}-\frac{1}{1320}+\frac{1}{9360}-\frac{1}{75600}+\cdots$$

c) Find the number of terms needed in a Taylor polynomial to have an error of less than 0.0001.

Since the Taylor polynomial is an alternating series, the Alternating Series Estimation Theorem can be used to determine the number of terms to include in the series [4].

If $s=\sum(-1)^{n-1}b_n$ is the sum of an alternating series that satisfies

- $b_{n+1}\le b_n$ and
- $\lim\limits_{n\to\infty} b_n=0$,

then

$$|R_n|=|s-s_n|\le b_{n+1}.$$

Looking at the value of the 6th, 7th and 8th terms in the series,

$$\frac{1}{1320} = 0.0007576$$

$$\frac{1}{9360} = 0.00011068$$

$$\frac{1}{75600} = 0.0000132$$

we see that 7 terms are need to achieve the desired accuracy.

$$\int_0^1 e^{-x^2}\,dx = 0.7468360343$$

Part III Writing MATLAB Code

4. MATLAB code to evaluate $\int_0^{\pi} \sin(x)\,dx$ using Simpson's Rule is given below.

5. Modify the code by changing the necessary lines of the program to do the following:

- Change the function from sin(x) to e^{-x^2}. **Note**: e^{x^2} in MATLAB is written as exp(x.^2).
- Change the limits of integration to match the limits for $\int_0^1 e^{-x^2}\,dx$.

Modified code with comments.

```
% simpsonint.m
% Evaluates the integral of a function over an interval
% input: function f(x) = exp(-x^2)
%        limits of integration: a – lower limit; b – upper limit
% output: the value of the integral

format long  % display numbers in the long fixed-decimal format
clear        % removes all variables from the current workspace
a=0;         % lower limit of integration
b=1;         %  upper limit of integration
% enter the number of intervals from the keyboard
n=input('input number of intervals (n must be an even number) ->');
```

```
h = (b-a)/n;  %  width of interval

fa = exp(-a.^2); % f(a)- function value at left endpoint
fb = exp(-b.^2);   % f(b)- function value at right endpoint

fsum=0;  % the area of each interval will be stored in fsum. Start with 0 area

for i = 2:2:n;  % all 4*f(a+nh) terms to f(b) h = (1,3,5,7,...,n-1)
   x = (a+(i-1)*h); % find x-value of all terms multiplied by 4
   fx = exp(-x.^2);  % evaluate function at each x-value
   fsum = fsum + 4*fx; % add to current sum
end

for i = 3:2:n;  % all 2*f(a+nh) terms to f(b) h = (2,4,6,...,n-2)
   x = (a+(i-1)*h);  % find x-value of all terms multiplied by 2
   fx = exp(-x.^2);  % evaluate function at each x-value
   fsum = fsum + 2*fx;  % add to current sum
end

result = (h/3)*(fa+fb+fsum)  % find area
```

Part IV Use MATLAB to evaluate the integral, $\int_0^1 e^{-x^2}\,dx.$

The exact value of the integral is assumed to be the value calculated using the **integral** command. The value of the integral is calculated using the following code.

```
syms x
format long
fun= @ (x)exp(-x.^2);
q=integral(fun,0,1)

q = 0.746824132812427
```

Table 1 Error Using Simpson's Rule

n (number of intervals)	Value of integral	Error
2	0.747180428909510	-0.00035629
4	0.746855379790987	-0.00060312
6	0.746830391489345	-0.00000626

Taylor polynomial code

```
syms x
expr = exp(-x.^2); % state function
texpr = taylor(expr, 'Order', 8)    % get the terms in the Taylor series
int(texpr,x ,0,1)   % integrate terms in Taylor series
```

Table 2 Error Using Taylor Polynomials

n (number of terms)	Value of integral	Error
5	0.747486772486773	-0.00066264
6	0.746729196729197	0.00009494
7	0.746836034336034	-0.00001190
8	0.746822806822807	0.00000133