Problem 1.

(30 points)

- (a) Use the forward-difference and backward-difference formulas to determine each missing entry in the following table with $f(x) = \sin x$, compute the errors and find error bounds using error formulas.
- (b) Choose your favorite function f, nonzero number x. Generate approximations of $f'_n(x)$ to f'(x) by

$$f'_n(x) = \frac{f(x+10^{-n}) - f(x)}{10^{-n}}$$

for n = 1, 2, ..., 10 and describe what happens.

Solution

Part (a)

x	f(x)	f'(x)	$\cos x$	$\varepsilon = \cos x - f'(x) $
0.5	0.4794	0.85200	0.87758	0.025580
0.6	0.5646	0.79600	0.82534	0.029340
0.7	0.6442	0.79600	0.76484	0.031160

We find the error term $\left| \frac{h}{2} f''(\xi) \right|$ from the following formula

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2}f''(\xi)$$

This error bound will be the same for forward and backward difference. We have $f''(x) = -\sin x$ and h = 0.1 in all cases, thus our error is given by $\lfloor \frac{0.1}{2} \sin \xi \rfloor$ where ξ is a value within the bounds of our difference. For each, we therefore want to maximize the value $\sin \xi$.

f'(0.5): $max_{0.5,0.6} \sin \xi = 0.564642 \Rightarrow = \frac{0.1}{2}0.564642 = 0.028232$ Thus we have an error bound of 0.02832 which is just a bit over our actual error of 0.025580.

f'(0.6): $max_{0.6,0.7} \sin \xi = 0.644218 \Rightarrow = \frac{0.1}{2}0.644218 = 0.03221$ Thus we have an error bound of 0.03221 a little bit worse than before. Our actual error of 0.029340 fits nicely within this bound.

f'(0.7): $max_{0.6,0.7} \sin \xi = 0.644218 \Rightarrow = \frac{0.1}{2}0.644218 = 0.03221$ Since we are taking the backward difference, we come to the same error bound as the forward difference for f'(0.6), that is 0.03221. Our actual error for this value is the worst at 0.031160 but still within the error bounds like we would expect.

Part (b)

Let $f(x) = \sin(x)$, and x = 3. We have $f'(x) = \cos(x)$, thus $f'(3) = \cos(3) = -0.9899924966$.

n	$f_n'(x)$	$ f'_n(x) - f'(x) $
1	-0.995393456265767	0.005400959665322
2	-0.990681590968298	0.000689094367853
3	-0.990062891599724	0.000070394999279
4	-0.989999550952969	0.000007054352524
5	-0.989993202188399	0.000000705587954
6	-0.989992567285158	0.000000070684713
7	-0.989992501865267	0.000000005264821
8	-0.989992490763036	0.000000005837409
9	-0.989992560151975	0.000000063551530
10	-0.989992532396400	0.000000035795954

In general, for larger values of n we would expect the error between our approximation and the actual derivative to go down. However, if we in the above example we can see the error actually increase from n=7 to n=8 and from n=8 to n=9. We do see a decrease again from n=9 to n=10 however we still don't have the precision found at n=7 right before our estimates started to get worse.

Problem 2.

(60 points)

(a) Approximate the following integral using the Trapezoidal rule, find a bound for the error using error formula and compare this to the actual error:

$$\int_{0.5}^{1} x^4 dx$$
.

- (b) Repeat part (a) using Simpson's rule.
- (c) Repeat part (a) using Composite Trapezoidal rule with n=4.
- (d) Repeat part (a) using Composite Simpson rule with n = 4.
- (e) Write a code to implement part (c) and (d) in MATLAB.
- (f) Write a function v = CompositeTrapezoidalRule(f, a, b, n) to implement Composite trapezoidal rule with a given n for

$$\int_{a}^{b} f(x)dx,$$

verify your code with part (c).

Solution

Part (a)

By the trapezoidal rule, our approximation is given by $\frac{h}{2}[f(x_0) + f(x_1)]$. Where $x_0 = 0.5, x_1 = 1$ gives us $f(x_0) = 0.0625, f(x_1) = 1.0$. The estimate is given by $1.0625\frac{0.5}{2} = 0.26562$. The actual value of the integral is 0.19375, thus our actual error is |0.26562 - 0.19375| = 0.071875.

The trapezoidal rule has an error term of $\frac{h^3}{12}f''(\xi)$. Where $f''(\xi) = 12\xi^2$, maximizing this on the bounds (0.5, 1) gives us 12, thus our error bound $= \frac{0.5^3}{12}12 = 0.5^3 = 0.125$. Note that our actual error 0.071875 is within this error bound.

Part (b)

First we compute the values needed by Simpson's rule. We have a=0.5, b=1.0 thus $h=(1.0-0.5)/2=0.25, x_0=a=0.5, x_1=a+h=0.75, x_2=1.0$. Simpson's rule is given by $\frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)]$, filling in our values gives us $\frac{0.25}{3}[0.5^4+4\times0.75^4+1^4]=0.08333[0.0625+1.2656+1]=0.08333[2.3281]=0.194$. Given the actual value of the integral as 0.19375 our actual error is then |0.194-0.19375|=0.00025057.

Simpson's rule has an error term of $\frac{h^5}{90}f^{(4)}(\xi)$. Where $f^{(4)}(\xi) = 24$. Our error bound is then $24\frac{0.25^5}{90} = 0.00026042$. Our actual error sneaks just under this error bound.

Part (c)

For Composite Trapezoidal Rule with n=4, we have $h=(1.0-0.5)/4=0.125, x_i=[0.5,0.625,0.75,0.875,1.0], i\in[0,1,\ldots,4]$. The Composite Trapezoidal Approximation is given by $\frac{h}{2}[f(a)+2\sum_{j=1}^{n-1}f(x_j)+f(b)]$. Plugging in our values gives us

$$\int_{0.5}^{1} x^4 dx \approx \frac{0.125}{2} [f(0.5) + 2(f(0.625) + f(0.75) + f(0.875)) + f(1.0)]$$

$$= \frac{0.125}{2} [0.0625 + 2(1.0557) + 1]$$

$$= \frac{0.125}{2} [3.1739]$$

$$= 0.19837$$

With an actual value of 0.19375 our actual error is 0.19837 - 0.19375 = 0.0046188.

The error term is given by $\frac{b-a}{12}h^2f''(\mu)$. From part (a) we know we can maximize $f''(\mu)$ as 12. Thus the error bound is $12\frac{1-0.5}{12}0.125^2=0.0078125$. Again, our actual is nicely within this bound.

Part (d)

For Composite Simpson's Rule with n=4, we have $h=(1.0-0.5)/4=0.125, x_i=[0.5,0.625,0.75,0.875,1.0], i\in[0,1,\ldots,4]$, these are the same values obtained from Composite Trapezoidal Rule. The desired approximation is given by $\frac{h}{3}[f(a)+2\sum_{j=1}^{(n/2)-1}f(x_{2j})+4\sum_{j=1}^{n/2}f(x_{2j-1})+f(b)]$. Plugging in our values gives us

$$\begin{split} \int_{0.5}^{1} x^4 dx \approx & \frac{0.125}{3} [f(0.5) + 2(f(0.75)) + 4(f(0.625) + f(0.875)) + f(1.0)] \\ = & \frac{0.125}{3} [0.625 + 2(0.31641) + 4(0.73877) + 1.0] \\ = & \frac{0.125}{3} [4.6504] \\ = & 0.193766276 \end{split}$$

With an actual value of 0.19375 our actual error is 0.193766276 - 0.19375 = 0.0000162760416666519.

The error term is given by $\frac{b-a}{180}h^4f^{(4)}(\mu)$. From part (b) we know we $f^{(4)}(\mu) = 24$. Putting it all together yields $24\frac{1.0-0.5}{180}0.125^4 = 0.0000162760416666667$. Here we have a pretty accurate error bound and our actual value is falling just under it, though at this number of significant digits we might expect computer precision to be affecting our results.

Part (e)

For CompositeTrapezoidalRule see my answer to part (f).

```
function v = CompositeSimpsonsRule(f, a, b, n)
        h = (b-a)/n;
        x = (a+h):h:b;
        i = 1:((n/2)-1);
        j = 1:(n/2);
        part1 = 2 * sum(f(x(2.*i)));
        part2 = 4 * sum(f(x(2.*j-1)));
        inner = f(a) + part1 + part2 + f(b);
        v = (h/3) * inner;
end
Running
                CompositeSimpsonsRule(@(x)x.^4, 0.5, 1, 4)
produces a result of 0.19377 which is the same I found in part (d).
Part (f)
function v = CompositeTrapezoidalRule(f, a, b, n)
        h = (b-a)/n;
        x = (a+h):h:b;
        j = 1:(n-1);
        part = 2 * sum(f(x(j)));
        inner = f(a) + part + f(b);
        v = (h/2) * inner;
end
Running
```

 $CompositeTrapezoidalRule(@(x)x.^4, 0.5, 1, 4)$

produces a result of 0.19830 which is roughly the same I found in part (c). There is some variation at later significant digits, but I would attribute to truncation when computing by hand.

Problem 3.

(20 points)

(a) Show that the following quadrature formula has a degree of precision equal to 3,

$$\int_{-1}^{1} f(x)dx = f(-\frac{\sqrt{3}}{3}) + f(\frac{\sqrt{3}}{3}).$$

(b) Approximate the following integral using Gaussian quadrature with n = 2, 3, 5,

$$\int_{1}^{1.5} x^2 \ln x dx$$

Solution

Part (a)

Proof. If the quadrature formula has a degree of precision equal to 3, then x^k must be exact for each k = 0, 1, 2, 3. Further 3 must be the largest integer for which this is true. Thus if it is in fact true for k = 0, 1, 2, 3 (as we will show), it then must not be true for k = 4 else the quadrature formula would have a degree of precision equal to 4.

k=0: $\int_{-1}^{1} x^0 dx = \int_{-1}^{1} dx = 2$, further $\left(-\frac{\sqrt{3}}{3}\right)^0 + \frac{\sqrt{3}}{3} = 1 + 1 = 2$. Therefore we have at least a quadrature with degree of precision 0.

k=1: $\int_{-1}^{1} x dx = 0$, further $\left(-\frac{\sqrt{3}}{3}\right) + \frac{\sqrt{3}}{3}\right) = 0 \Rightarrow$ our degree of precision is at least 1.

k=2: $\int_{-1}^{1} x^2 dx = \frac{2}{3}$, further $(-\frac{\sqrt{3}}{3})^2 + \frac{\sqrt{3}}{3})^2 = \frac{1}{3} + \frac{1}{3} = \frac{2}{3} \Rightarrow$ our degree of precision is at least 2.

k=3: $\int_{-1}^{1} x^3 dx = 0$, further $(-\frac{\sqrt{3}}{3})^3 + \frac{\sqrt{3}}{3})^3 = -(\frac{\sqrt{3}}{3})^3 + \frac{\sqrt{3}}{3})^3 = 0 \Rightarrow$ our degree of precision is at least 3.

k=4: $\int_{-1}^{1} x^2 dx = \frac{4}{10}$, further $(-\frac{\sqrt{3}}{3})^4 + \frac{\sqrt{3}}{3})^4 = 2(\frac{\sqrt{3}}{3})^4 = 2\frac{9}{81} = 2\frac{1}{9} = \frac{2}{9}$. But as $\frac{4}{10} \neq \frac{2}{9} \Rightarrow$ our degree of precision is less than 4.

Note that by a generalization of the argument provided for k=3 we know that the quadrature formula will be true for all odd k, but for a degree of precision of k we need it to be true for all integers less than or equal to k. Thus as the formula is not exact at k=4 and is exact for k=0,1,2,3 we know that we must have a degree of precision equal to 3.

Part (b)

Before we begin, we must first transform the given integral on the bounds 1, 1.5 to the bounds -1, 1 through the following transformation

$$\int_{1}^{1.5} f(x)dx = \int_{-1}^{1} f\left(\frac{(1.5-1)t+1+1.5}{2}\right) \frac{(1.5-1)}{2}dt$$
$$= \int_{-1}^{1} f\left(\frac{0.5t+2.5}{2}\right) 0.25dt$$
$$= \int_{-1}^{1} 0.25f(0.25t+1.25)dt$$

Thus define g(x) = 0.25 f(0.25x + 1.25). Therefore the approximation via Gaussian quadrature is given by $\sum_{i=1}^{n} c_i g(x_i)$. Note that the actual value of the integral we are approximating is 0.192259.

n=2:

From the table in the lecture notes c = [1.0, 1.0]. The points we would like to consider are $x_i = [-1, 1]$, plugging these into the formula above gives us

$$\int_{1}^{1.5} x^{2} \ln x dx \approx c_{1}g(x_{1}) + c_{2}g(x_{2})$$

$$= g(-1) + g(1)$$

$$= 0.22807$$

This is an error of 0.035811.

n=3:

From the table in the lecture notes $c = [\frac{5}{9}, \frac{8}{9}, \frac{5}{9}]$. The points we would like to consider are $x_i = [-1, 0, 1]$, plugging these into the formula above gives us

$$\int_{1}^{1.5} x^{2} \ln x dx \approx c_{1}g(x_{1}) + c_{2}g(x_{2}) + c_{3}g(x_{3})$$

$$= \frac{5}{9}g(-1) + \frac{8}{9}g(0) + \frac{5}{9}g(1)$$

$$= 0.0 + 0.07748 + 1.2671$$

$$= 0.20419$$

This is an error of 0.011931.

n=5:

From the table in the lecture notes

c = [0.2369268850, 0.4786286705, 0.5688888889, 0.4786286705, 0.2369268850]. The points we would like to consider are $x_i = [-1, -0.5, 0, 0.5, 1]$, plugging these into the formula above gives us

$$\int_{1}^{1.5} x^{2} \ln x dx \approx c_{1}g(x_{1}) + c_{2}g(x_{2}) + c_{3}g(x_{3}) + c_{4}g(x_{4}) + c_{5}g(x_{5})$$

$$= 0.2369268850g(-1.0) + 0.4786286705g(-0.5) + 0.5688888889g(0.0) + 0.4786286705g(0.5) + 0.2369268850g(1.0)$$

$$= 0.000000 + 0.017837 + 0.049587 + 0.072043 + 0.054037$$

$$= 0.19350$$

This is an error of 0.0012410.

We can see that as we increase n we get a more accurate approximation of the actual integral.

Problem 4.

(20 points)

(a) Use Composite Simpson rule with n=4 to approximate the following integral

$$\int_0^1 x^{-1/4} \sin x dx$$

(b) Use Composite Simpson rule with n=6 to approximate the following integral

$$\int_{1}^{\infty} \frac{\cos x}{x^3} dx$$

Solution

Part (a)

We have values a = 0, b = 1, n = 4 from this we can derive h = (b - a)/n = 0.25. With points $x_i = [0, 0.25, 0.5, 0.75, 1.0], i \in [0, 1, ..., 4]$.

Note that $x^{-1/4} \sin x$ has a singularity at it's left endpoint, even though the integral exists. We can get around this by first computing the fourth Taylor Polynomial P_4 for $g(x) = \sin x$.

$$P_4(x) = g(0) + g'(0)(x) + \frac{g''(0)}{2}(x)^2 + \frac{g'''(0)}{6}(x)^3 + \frac{g^{(4)}}{24}(x)^4$$
$$= 0 + x + 0 + \frac{-x^4}{24} = x + \frac{-x^4}{24}$$

We now write

$$\int_0^1 \frac{\sin x}{x^{1/4}} dx = \int_0^1 \frac{\sin(x) - (x + \frac{-x^4}{24})}{x^{1/4}} dx + \int_0^1 \frac{x + \frac{-x^4}{24}}{x^{1/4}}$$

Note that the second integral above is an integral over a polynomial, we can compute this exactly as 0.56266. Thus we now have

$$\int_0^1 \frac{\sin x}{x^{1/4}} dx = \int_0^1 \frac{\sin(x) - (x + \frac{-x^4}{24})}{x^{1/4}} dx + 0.56266$$

We now define G(x) and use Composite Simpson's rule on [0,1] to evaluate the remaining integral.

$$G(x) = \begin{cases} 0 & \text{if } x = 0\\ \frac{\sin(x) - (x + \frac{-x^4}{24})}{x^{1/4}} & \text{otherwise} \end{cases}$$

The approximation by Composite Simpson's Rule on G(x) is given by $\frac{h}{3}[G(a) + 2\sum_{j=1}^{(n/2)-1}G(x_{2j}) + 4\sum_{j=1}^{n/2}G(x_{2j-1}) + G(b)].$ Plugging in our values gives us

$$\int_0^1 x^{-1/4} \sin x dx \approx \frac{0.25}{3} [G(a) + 2(G(x_2)) + 4(G(x_1) + G(x_3)) + G(b)]$$

$$= \frac{1}{12} [G(0) + 2(G(0.5)) + 4(G(0.25) + G(0.75)) + G(1)]$$

$$= \frac{1}{12} [0 - 0.042741 - 0.25093 - 11686]$$

$$= \frac{1}{12} [-0.41054]$$

$$= -0.034211$$

Putting it all together and we arrive at

$$\int_0^1 \frac{\sin x}{x^{1/4}} dx \approx -0.034211 + 0.56266 = 0.52845$$

This is not too far off from the actual value of 0.56266 with an actual error of 0.034211.

Part (b)

We can convert this right endpoint of infinity into a limit with a left endpoint singularity at 0 via the following substitution

$$\int_{a}^{\infty} f(x)dx = \int_{0}^{1/a} t^{-2} f(\frac{1}{t})dt$$

In this particular instance we have $f(x) = \frac{\cos x}{x^3}$ giving us the following integral to solve $\int_0^1 t^{-2} \frac{\cos(1/t)}{(1/t)^3} dt = \int_0^1 t \cos(1/t)$.

Problem 5.

(30 points)

(a) Use the Gaussian Elimination with Backward substitution to solve the following linear system (must show intermediate steps).

$$2x_1 - 1.5x_2 + 3x_3 = 1$$

$$-x_1 + 2x_3 = 3$$

$$4x_1 - 4.5x_2 + 5x_3 = 1$$

- (b) Repeat (a) using the Gaussian Elimination with partial pivoting and Backward substitution (must show intermediate steps).
- (c) Repeat (a) using Gaussian Elimination with scaled partial pivoting and Backward substitution (must show intermediate steps).

Solution

Problem 6.

(20 points)

(a) Solve the following linear system with forward and backward substitution,

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 3 & -1 \\ 0 & -2 & 1 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ -1 \\ 1 \end{bmatrix}$$

(b) Use the LU factorization (no permutation) with forward and backward substitution to solve the following linear system (Use the sample MATLAB codes posted on classpage as discussed in class),

$$2x_1 + 3x_2 - x_3 = 2$$
$$4x_1 + 4x_2 - x_3 = -1$$
$$-2x_1 - 3x_2 + 4x_3 = 1$$

Solution

Problem 7.

(20 points)

(a) Use the $A = LDL^t$ factorization to solve the following linear system,

$$2x_1 - x_2 = 2$$

$$-x_1 + 2x_2 - x_3 = -1$$

$$-x_2 + 2x_3 = 1$$

(b) Repeat (a) with Cholesky factorization $A=LL^t$.

Solution