AME 60614: Numerical Methods
Fall 2007, Problem Set 1 Solutions

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1. *The following discrete data points were obtained from an unknown function $f(x)$.*

n	x_n	$f(x_n)$	n	x_n	$f(x_n)$
1	-4.0000	-0.1245	10	0.0625	0.4706
2	-3.0625	-0.1622	11	0.2500	1.0000
3	-2.2500	-0.2195	12	0.5625	0.7423
4	-1.5625	-0.3120	13	1.0000	0.4706
5	-1.0000	-0.4706	14	1.5625	0.3120
6	-0.5625	-0.7423	15	2.2500	0.2195
7	-0.2500	-1.0000	16	3.0625	0.1622
8	-0.0625	-0.4706	17	4.0000	0.1245
9	0.0000	0.0000			

(a) *Plot the points and draw your best guess of an interpolation of the function.*

(b) *Show a Lagrange interpolation of the function using all of the points.*

(c) *Show a Lagrange interpolation of the function using only the even points, then only the odd points.*

(d) *Show piecewise Lagrange interpolations, first linear then on three subsets of the points. (i.e. n = 1-7, 7-11, 11-17)*

(e) *Show a cubic spline interpolation of the function. Show two different values of tension on the cubic spline.*

Submit one labeled graph for each part and comment on each.

(a)

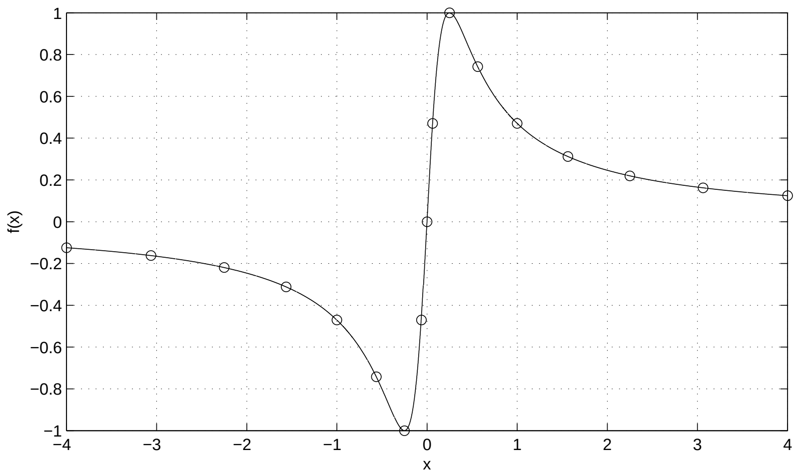

Figure 1: Actual Function

The actual function that the points were plotting is $f(x) = \frac{8x}{16x^2+1}$, which is shown in figure 1. An intuitive interpolation of this function would probably look similar to this.

(b) To obtain the coefficients for the Lagrange interpolating polynomial a system of N equations is set up with the coefficients being the N unknowns. This system looks like

$$
\begin{bmatrix}
x_1^0 & x_1^1 & x_1^2 & & x_1^{N-1} & x_1^N \\
x_2^0 & x_2^1 & x_2^2 & \dots & x_2^{N-1} & x_2^N \\
x_3^0 & x_3^1 & x_3^2 & & x_3^{N-1} & x_3^N \\
 & \vdots & & \ddots & & \vdots \\
x_{N-1}^0 & x_{N-1}^1 & x_{N-1}^2 & & x_{N-1}^{N-1} & x_{N-1}^N \\
x_N^0 & x_2^1 & x_N^2 & \dots & x_N^{N-1} & x_N^N
\end{bmatrix}
\begin{bmatrix}
a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{N-2} \\ a_{N-1}
\end{bmatrix}
=
\begin{bmatrix}
f(x_1) \\ f(x_2) \\ f(x_3) \\ \vdots \\ f(x_{N-1}) \\ f(x_N)
\end{bmatrix}.
$$

Plugging in the x and $f(x)$ values and solving for the a values yields the Lagrange Interpolating Polynomial of the form

$$f_L(x) = a_{N-1}x^{N-1} + a_{N-2}x^{N-2} + \dots a_2x^2 + a_1x + a_0$$

which can be seen in figure 2. Note that despite passing through every point, which is guaranteed

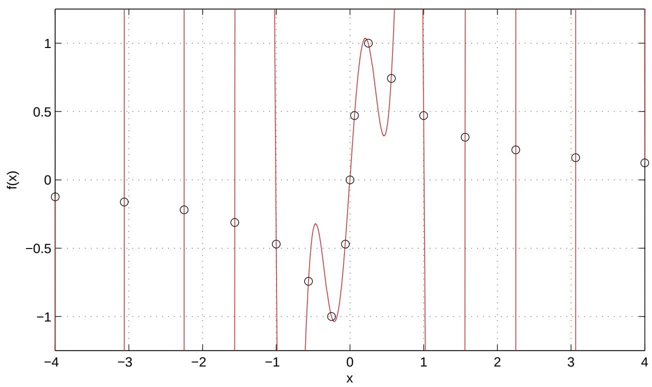

Figure 2: Lagrange Interpolating Polynomial: All 17 Points

by solving the system, the polynomial does not accurately interpolate between the points and has excessive error $O(10^6)$. You may have noticed that the points indicate the function is an odd function. This is also shown by the coefficients in the Lagrange interpolating polynomial being zero for all of the even exponents of x. It is interesting to note that one can use either all the positive points or all the negative points or even a unique combination of the two of them, along with the knowledge that the function is odd (i.e. only including odd exponents) to yield exactly the same interpolating polynomial. For this you must either not include the point $x_i = 0$ (which is implicitly zero with an odd function assumption), or include the constant term (an even term) to keep the matrix displayed above non-singular.

(c) Cutting the number of points approximately in half and solving the same equation for the Lagrange Interpolating Polynomial still produces large errors as shown in figure 3, but the error is reduced to $O(10^2)$ which is a vast improvement over using a Lagrange Interpolation for all 17 points.

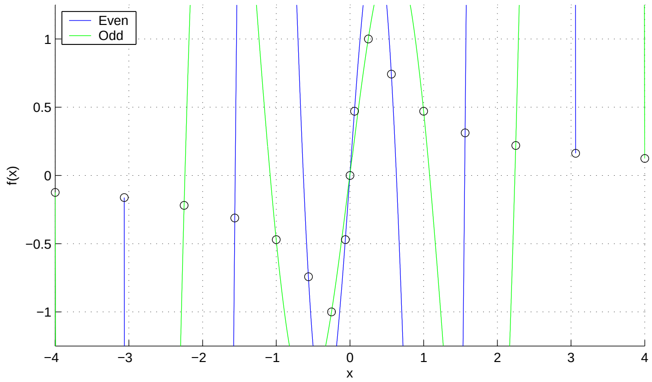

Figure 3: Lagrange Interpolating Polynomial: Half the Points

(d) The trend of improvement for interpolation with the reduction of the number of points continues and is shown in figure 4. The linear and three segment interpolations match much better to the function than did the interpolations from section (b) or (c). The error has been reduced in this case to $O(10^{-1})$. A drawback to using this method is that the derivatives of the interpolation are not continuous between the segments.

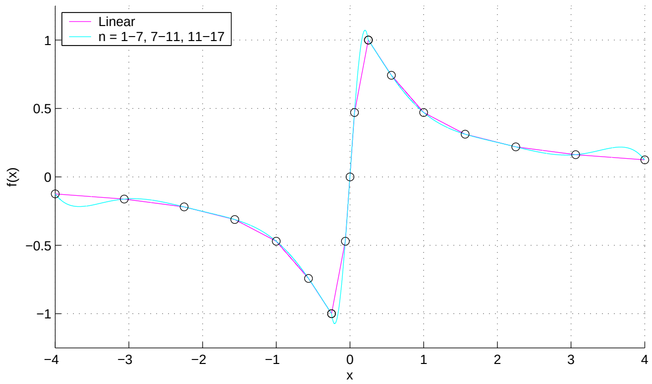

Figure 4: Lagrange Interpolating Polynomial: Piecewise Linear and Three Segment

(e) One way to avoid the discontinuities in derivatives is to force them to be continuous, which is what is done in the cubic spline, which is shown in figure 5. Every segment of the cubic spline is piecewise continuous for the functional value as well as the first and second derivatives. To solve for the cubic spline, a tridiagonal system is set up for the second derivative values at each point given by the $N-2$ equations

$$\frac{h_{i-1}}{6}f''(x_{i-1}) + \frac{h_{i-1}+h_i}{3}f''(x_{i-1}) + \frac{h_i}{6}f''(x_{i+1}) = \frac{f(x_{i+1})-f(x_i)}{h_i} - \frac{f(x_i)-f(x_{i-1})}{h_{i-1}},$$

along with the two boundary conditions, which for this case are appropriate to be free boundary conditions

$$f''(x_1) = f''(x_N) = 0.$$

This tridiagonal system ends up looking like

$$\begin{bmatrix} 1 & & & & & & \\ h_1 & 2(h_1+h_2) & h_2 & & & & \\ & h_2 & 2(h_2+h_3) & h_3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & h_{N-2} & 2(h_{N-2}+h_{N-1}) & h_{N-1} & \\ & & & & h_{N-1} & 2(h_{N-1}+h_N) & h_N \\ & & & & & & 1 \end{bmatrix} \begin{bmatrix} f''_1 \\ f''_2 \\ \\ \vdots \\ \\ f''_{N-1} \\ f''_N \end{bmatrix}$$

$$= 6 \begin{bmatrix} 0 \\ \frac{f_3-f_2}{h_2} - \frac{f_2-f_1}{h_1} \\ \\ \vdots \\ \\ \frac{f_{N-2}-f_{N-1}}{h_{N-1}} - \frac{f_{N-1}-f_N}{h_N} \\ 0 \end{bmatrix},$$

Figure 5 also shows two values of tension, $\sigma = 25$ and $\sigma = 750$, which are solved in a similar manner to the non-tension cubic spline. The higher the tension, the straighter the line.

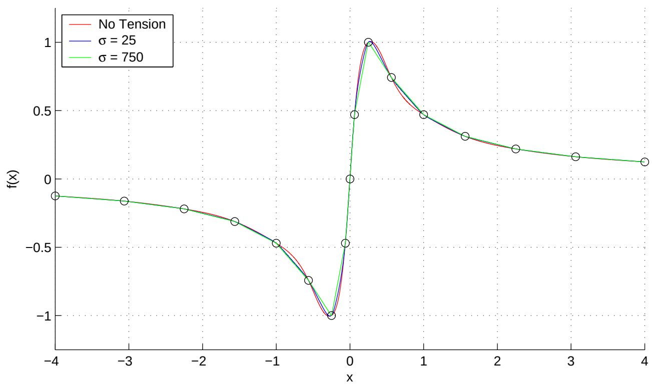

Figure 5: Cubic Spline: Tension and No Tension

2. *Interpolate the ellipse given by the equation $x^2+4y^2=4$ using a parametric cubic spline with $N=4$, 8, and 16, unique and approximately evenly spaced points. How many points do you have to use to apply appropriate boundary conditions? Now, see how rapidly the error converges to zero as you increase N. Plot the maximum error of the interpolation against the number of points on a* log-log *scale. Be sure to include enough data points to verify this trend up to a very large value of N. How small an error can you attain?*

   To set up a parametric cubic spline, a parametric equation for the ellipse must first be found. A simple solution is

$$\begin{aligned} x(s) &= 2\sin(s), \\ y(s) &= \cos(s), \\ s &\in [0, 2\pi). \end{aligned}$$

   From this parametric equation, two cubic splines are necessary: one for $x(s)$ and one for $y(s)$. The variable s is then broken into N equally spaced and unique points (i.e. $s=\frac{2n\pi}{N}$). To apply the periodic boundary conditions $x_0''(s)=x_{M-1}''(s)$ and $x_1''(s)=x_M''(s)$ (only shown in x, but the same applies to y), the first point must overlap the second to last point and the second point must overlap the last point. This means that for N unique points $M=N+2$, and therefore

$$s=\frac{2n\pi}{N} \qquad \text{where} \qquad n=0,1,\dots,N,N+1.$$

   With s equally spaced, then $h_i=h=\frac{2\pi}{N}$ and the tridiagonal system then has constant coefficients, and with the boundary conditions it is formatted

$$\begin{bmatrix} 1 & 0 & 0 & \dots & 0 & -1 & 0 \\ h & 4h & h & & & & \\ & h & 4h & h & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & h & 4h & h & \\ & & & & h & 4h & h \\ 0 & -1 & 0 & \dots & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_0''(s) & y_0''(s) \\ x_1''(s) & y_1''(s) \\ & \\ \vdots & \vdots \\ & \\ x_N''(s) & y_N''(s) \\ x_{N+1}''(s) & y_{N+1}''(s) \end{bmatrix} = \frac{6}{h} \begin{bmatrix} 0 & 0 \\ \delta^2 x_1(s) & \delta^2 y_1(s) \\ \delta^2 x_2(s) & \delta^2 y_2(s) \\ \vdots & \vdots \\ \delta^2 x_{N-1}(s) & \delta^2 y_{N-1}(s) \\ \delta^2 x_N(s) & \delta^2 y_N(s) \\ 0 & 0 \end{bmatrix},$$

   where the δ^2 is the central difference operator. This can be solved directly or reduced into the following periodic tridiagonal matrix

$$\begin{bmatrix} 4h & h & & & h \\ h & 4h & h & & \\ & \ddots & \ddots & \ddots & \\ & & h & 4h & h \\ h & & & h & 4h \end{bmatrix} \begin{bmatrix} x_1''(s) & y_1''(s) \\ x_2''(s) & y_2''(s) \\ \vdots & \vdots \\ x_{N-1}''(s) & y_{N-1}''(s) \\ x_N''(s) & y_N''(s) \end{bmatrix} = \frac{6}{h} \begin{bmatrix} \delta^2 x_1(s) & \delta^2 y_1(s) \\ \delta^2 x_2(s) & \delta^2 y_2(s) \\ \vdots & \vdots \\ \delta^2 x_{N-1}(s) & \delta^2 y_{N-1}(s) \\ \delta^2 x_N(s) & \delta^2 y_N(s) \end{bmatrix},$$

   which is computationally less costly to solve using the Sherman-Morrison Formula and Thomas Algorithm. The second derivative values at 0 and $N+1$ that were eliminated from the reduced periodic tridiagonal system are found by directly applying the periodic boundary conditions after the solution is obtained. The parametric equation is then obtained for both

$$\begin{aligned} x_i(s) &= \tfrac{(s_{i+1}-s)^3 x''(s_i)+(s-s_i)^3 x''(s_{i+1})}{6h} + (s_{i+1}-s)\left(\tfrac{x(s_i)}{h}-\tfrac{h}{6}x''(s_i)\right) + (s-s_i)\left(\tfrac{x(s_{i+1})}{h}-\tfrac{h}{6}x''(s_{i+1})\right), \\ y_i(s) &= \tfrac{(s_{i+1}-s)^3 y''(s_i)+(s-s_i)^3 y''(s_{i+1})}{6h} + (s_{i+1}-s)\left(\tfrac{y(s_i)}{h}-\tfrac{h}{6}y''(s_i)\right) + (s-s_i)\left(\tfrac{y(s_{i+1})}{h}-\tfrac{h}{6}y''(s_{i+1})\right), \end{aligned}$$

   and piecewise plotted $y(s)$ against $x(s)$ which is shown in figure 6 for $N=4$, 8, and 16. To obtain the error the spline's values of $x(s)$ and $y(s)$ are plugged into the equation of the ellipse to yield $E(s)=\left|x(s)^2+4y(s)^2-4\right|$. This procedure is repeated for increasing values of N and the maximum

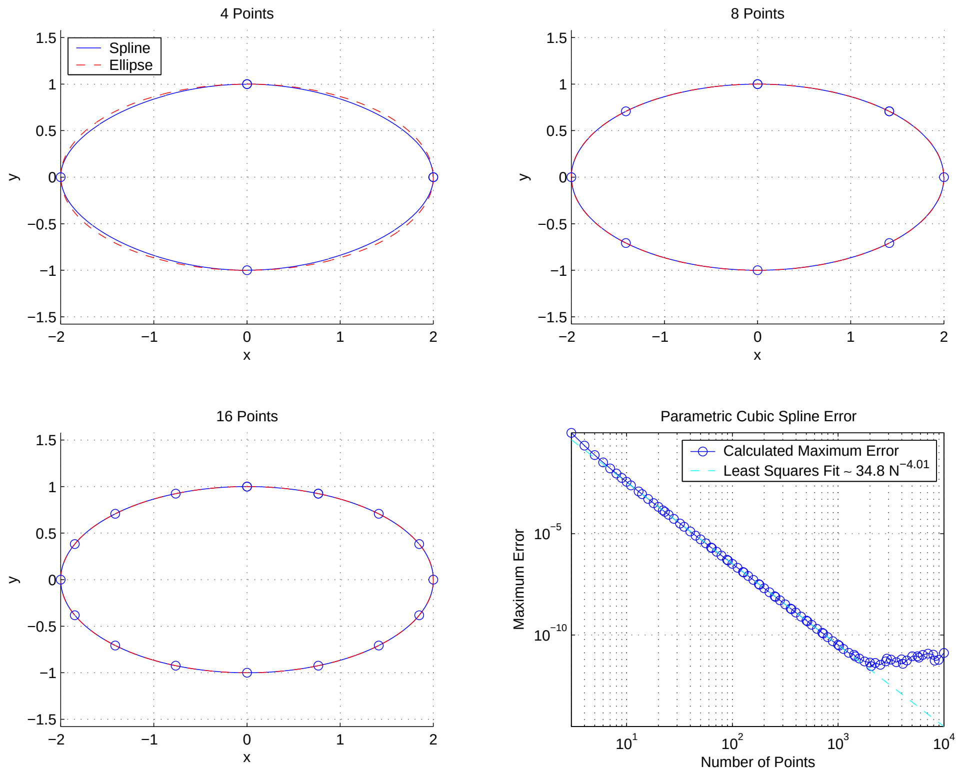

Figure 6: Parametric Cubic Spline and Maximum Error

value of this error is retained for each value of N and then plotted on a log-log scale in figure 6. This shows the the error decreases approximately with N^{-4} for values of N up to $O(10^3)$ when the machine precision begins to limit the convergence rate. The smallest maximum error that I was able to achieve was $E = 2.9345 \times 10^{-12}$, which was obtained at $N = 2048$.

3. *Find the most accurate finite difference formula and the corresponding leading error term for the following derivatives:*

   (a) $f''(x)$

   (b) $f^{(iv)}(x)$

   (c) $f'''(x) - 3f'(x)$

   to the highest order of accuracy possible using only the following function values.

   i f_{i-2}, f_{i-1}, f_i, f_{i+1}, *and* f_{i+2}

   ii f_i, f_{i+1}, f_{i+2}, f_{i+3}, *and* f_{i+4}

   iii f_{i-4}, f_{i-3}, f_{i-2}, f_{i-1}, *and* f_i

   iv f_{i-1}, f_i, f_{i+1}, f'_{i-1}, f'_i, *and* f'_{i+1}

   The solution to this problem is made simpler by creating a chart of the Taylor Series expansions of each of the terms for their respective derivatives

	f	f'	f''	f'''	$f^{(iv)}$	$f^{(v)}$	$f^{(vi)}$	$f^{(vii)}$
f_{i-4}	1	$-4h$	$8h^2$	$-\frac{32}{3}h^3$	$\frac{32}{3}h^4$	$-\frac{128}{15}h^5$	$\frac{256}{45}h^6$	$-\frac{1024}{315}h^7$
f_{i-3}	1	$-3h$	$\frac{9}{2}h^2$	$-\frac{9}{2}h^3$	$\frac{27}{8}h^4$	$-\frac{81}{40}h^5$	$\frac{81}{80}h^6$	$-\frac{243}{560}h^7$
f_{i-2}	1	$-2h$	$2h^2$	$-\frac{4}{3}h^3$	$\frac{2}{3}h^4$	$-\frac{4}{15}h^5$	$\frac{4}{45}h^6$	$-\frac{8}{315}h^7$
f_{i-1}	1	$-h$	$\frac{1}{2}h^2$	$-\frac{1}{6}h^3$	$\frac{1}{24}h^4$	$-\frac{1}{120}h^5$	$\frac{1}{720}h^6$	$-\frac{1}{5040}h^7$
f_i	1	0	0	0	0	0	0	0
f_{i+1}	1	h	$\frac{1}{2}h^2$	$\frac{1}{6}h^3$	$\frac{1}{24}h^4$	$\frac{1}{120}h^5$	$\frac{1}{720}h^6$	$\frac{1}{5040}h^7$
f_{i+2}	1	$2h$	$2h^2$	$\frac{4}{3}h^3$	$\frac{2}{3}h^4$	$\frac{4}{15}h^5$	$\frac{4}{45}h^6$	$\frac{8}{315}h^7$
f_{i+3}	1	$3h$	$\frac{9}{2}h^2$	$\frac{9}{2}h^3$	$\frac{27}{8}h^4$	$\frac{81}{40}h^5$	$\frac{81}{80}h^6$	$\frac{243}{560}h^7$
f_{i+4}	1	$4h$	$8h^2$	$\frac{32}{3}h^3$	$\frac{32}{3}h^4$	$\frac{128}{15}h^5$	$\frac{256}{45}h^6$	$\frac{1024}{315}h^7$
f'_{i-1}	0	1	$-h$	$\frac{1}{2}h^2$	$-\frac{1}{6}h^3$	$\frac{1}{24}h^4$	$-\frac{1}{120}h^5$	$\frac{1}{720}h^6$
f'_i	0	1	0	0	0	0	0	0
f'_{i+1}	0	1	h	$\frac{1}{2}h^2$	$\frac{1}{6}h^3$	$\frac{1}{24}h^4$	$\frac{1}{120}h^5$	$\frac{1}{720}h^6$.

   From this chart the system $Ac = d$ can be formed where A is a square matrix that can be made which includes as many terms in the Taylor Series as there are function values to solve for, c is an unknown vectors of the coefficients of the function values, and d is a vector that indicates the derivative to be approximated. The vectors are for each part of the problem:

$$
\begin{array}{cccccc}
 & \text{(a)} & & \text{(b)} & & \text{(c)} \\
d = & \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, & & \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, & & \begin{bmatrix} 0 \\ -3 \\ 0 \\ 1 \end{bmatrix}.
\end{array}
$$

   These vectors are padded on the bottom with zeros to make them match the size of the matrix. This makes it so that using n functional values to approximate an m^{th} derivative, the finite difference formula is at least $O(h^{(n-m)})$.

The matrices for each set of functional values are

$$
A = \begin{array}{cc}
\underline{\text{i}} & \underline{\text{ii}} \\
\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ -2h & -h & 0 & h & 2h \\ 2h^2 & \frac{1}{2}h^2 & 0 & \frac{1}{2}h^2 & 2h^2 \\ -\frac{4}{3}h^3 & -\frac{1}{6}h^3 & 0 & \frac{1}{6}h^3 & \frac{4}{3}h^3 \\ \frac{2}{3}h^4 & \frac{1}{24}h^4 & 0 & \frac{1}{24}h^4 & \frac{2}{3}h^4 \end{bmatrix}, &
\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & h & 2h & 3h & 4h \\ 0 & \frac{1}{2}h^2 & 2h^2 & \frac{9}{2}h^2 & 8h^2 \\ 0 & \frac{1}{6}h^3 & \frac{4}{3}h^3 & \frac{9}{2}h^3 & \frac{32}{3}h^3 \\ 0 & \frac{1}{24}h^4 & \frac{2}{3}h^4 & \frac{27}{8}h^4 & \frac{32}{3}h^4 \end{bmatrix}, \\
\underline{\text{iii}} & \underline{\text{iv}} \\
\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ -4h & -3h & -2h & -h & 0 \\ 8h^2 & \frac{9}{2}h^2 & 2h^2 & \frac{1}{2}h^2 & 0 \\ -\frac{32}{3}h^3 & -\frac{9}{2}h^3 & -\frac{4}{3}h^3 & -\frac{1}{6}h^3 & 0 \\ \frac{32}{3}h^4 & \frac{27}{8}h^4 & \frac{2}{3}h^4 & \frac{1}{24}h^4 & 0 \end{bmatrix}, \text{ and} &
\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ -h & 0 & h & 1 & 1 & 1 \\ \frac{1}{2}h^2 & 0 & \frac{1}{2}h^2 & -h & 0 & h \\ -\frac{1}{6}h^3 & 0 & \frac{1}{6}h^3 & \frac{1}{2}h^2 & 0 & \frac{1}{2}h^2 \\ \frac{1}{24}h^4 & 0 & \frac{1}{24}h^4 & -\frac{1}{6}h^3 & 0 & \frac{1}{6}h^3 \\ -\frac{1}{120}h^5 & 0 & \frac{1}{120} & \frac{1}{24}h^4 & 0 & \frac{1}{24}h^4 \end{bmatrix}.
\end{array}
$$

Inverting these A matrices (I preformed this task in *matlab* using the *sym()* command for h) and multiplying them by the d vectors given above yields the coefficient vectors shown in this chart

	i	ii	iii	iv
(a)	$\begin{bmatrix} -\frac{1}{12h^2} \\ \frac{4}{3h^2} \\ -\frac{5}{2h^2} \\ \frac{4}{3h^2} \\ -\frac{1}{12h^2} \end{bmatrix}$	$\begin{bmatrix} \frac{35}{12h^2} \\ -\frac{26}{3h^2} \\ \frac{19}{2h^2} \\ -\frac{14}{3h^2} \\ \frac{11}{12h^2} \end{bmatrix}$	$\begin{bmatrix} \frac{11}{12h^2} \\ -\frac{14}{3h^2} \\ \frac{19}{2h^2} \\ -\frac{26}{3h^2} \\ \frac{35}{12h^2} \end{bmatrix}$	$\begin{bmatrix} \frac{2}{h^2} \\ -\frac{4}{h^2} \\ \frac{2}{h^2} \\ \frac{1}{2h} \\ 0 \\ -\frac{1}{2h} \end{bmatrix}$
(b)	$\begin{bmatrix} \frac{1}{h^4} \\ -\frac{4}{h^4} \\ \frac{6}{h^4} \\ -\frac{4}{h^4} \\ \frac{1}{h^4} \end{bmatrix}$	$\begin{bmatrix} \frac{1}{h^4} \\ -\frac{4}{h^4} \\ \frac{6}{h^4} \\ -\frac{4}{h^4} \\ \frac{1}{h^4} \end{bmatrix}$	$\begin{bmatrix} \frac{1}{h^4} \\ -\frac{4}{h^4} \\ \frac{6}{h^4} \\ -\frac{4}{h^4} \\ \frac{1}{h^4} \end{bmatrix}$	$\begin{bmatrix} -\frac{12}{h^4} \\ \frac{24}{h^4} \\ -\frac{12}{h^4} \\ -\frac{6}{h^3} \\ 0 \\ \frac{6}{h^3} \end{bmatrix}$
(c)	$\begin{bmatrix} -\frac{1}{4h} - \frac{1}{2h^3} \\ \frac{2}{h} + \frac{1}{h^3} \\ 0 \\ -\frac{2}{h} - \frac{1}{h^3} \\ \frac{1}{4h} + \frac{1}{2h^3} \end{bmatrix}$	$\begin{bmatrix} \frac{25}{4h} - \frac{5}{2h^3} \\ -\frac{12}{h} + \frac{9}{h^3} \\ \frac{9}{h} - \frac{12}{h^3} \\ -\frac{4}{h} + \frac{7}{h^3} \\ \frac{3}{4h} - \frac{3}{2h^3} \end{bmatrix}$	$\begin{bmatrix} -\frac{3}{4h} + \frac{3}{2h^3} \\ \frac{4}{h} - \frac{7}{h^3} \\ -\frac{9}{h} + \frac{12}{h^3} \\ \frac{12}{h} - \frac{9}{h^3} \\ -\frac{25}{4h} + \frac{5}{2h^3} \end{bmatrix}$	$\begin{bmatrix} -\frac{15}{2h^3} \\ 0 \\ \frac{15}{2h^3} \\ -\frac{3}{2h^2} \\ -3 - \frac{12}{h^2} \\ -\frac{3}{2h^2} \end{bmatrix}$.

These coefficient vectors can then be multiplied by modified A matrices that are extended to include higher order terms in the Taylor Expansions. This operation will yield the higher order error terms, and the leading order term can be identified. An example of this for part (a)i is shown here:

$$
\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ -2h & -h & 0 & h & 2h \\ 2h^2 & \frac{1}{2}h^2 & 0 & \frac{1}{2}h^2 & 2h^2 \\ -\frac{4}{3}h^3 & -\frac{1}{6}h^3 & 0 & \frac{1}{6}h^3 & \frac{4}{3}h^3 \\ \frac{2}{3}h^4 & \frac{1}{24}h^4 & 0 & \frac{1}{24}h^4 & \frac{2}{3}h^4 \\ -\frac{4}{15}h^5 & -\frac{1}{120}h^5 & 0 & \frac{1}{120}h^5 & \frac{4}{15}h^5 \\ \frac{4}{45}h^6 & \frac{1}{720}h^6 & 0 & \frac{1}{720}h^6 & \frac{4}{45}h^6 \end{bmatrix}
\begin{bmatrix} -\frac{1}{12h^2} \\ \frac{4}{3h^2} \\ -\frac{5}{2h^2} \\ \frac{4}{3h^2} \\ -\frac{1}{12h^2} \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ -\frac{h^4}{90} \end{bmatrix}.
$$

The finite difference formulas with the leading order error for each part of this problem are listed here:

(i)

	Finite Difference Formula	Leading Order Error
$f''(x)$	$\frac{-f_{i-2}+16f_{i-1}-30f_i+16f_{i+1}-f_{i+2}}{12h^2}$	$-\frac{h^4}{90}f^{(vi)}(x)$
$f^{(iv)}(x)$	$\frac{f_{i-2}-4f_{i-1}+6f_i-4f_{i+1}+f_{i+2}}{h^4}$	$+\frac{h^2}{6}f^{(vi)}(x)$
$f'''(x)-3f'(x)$	$\frac{-f_{i-2}+2f_{i-1}-2f_{i+1}+f_{i+2}}{2h^3}+\frac{-f_{i-2}+8f_{i-1}-8f_{i+1}+f_{i+2}}{4h}$	$+\frac{h^2}{4}f^{(v)}(x)$

(ii)

	Finite Difference Formula	Leading Order Error
$f''(x)$	$\frac{35f_i-104f_{i+1}+114f_{i+2}-56f_{i+3}+11f_{i+4}}{12h^2}$	$-\frac{5h^3}{6}f^{(v)}(x)$
$f^{(iv)}(x)$	$\frac{f_i-4f_{i+1}+6f_{i+2}-4f_{i+3}+f_{i+4}}{h^4}$	$+2hf^{(v)}(x)$
$f'''(x)-3f'(x)$	$\frac{-5f_i+18f_{i+1}-24f_{i+2}+14f_{i+3}-3f_{i+4}}{2h^3}+\frac{25f_i-48f_{i+1}+36f_{i+2}-16f_{i+3}+3f_{i+4}}{4h}$	$-\frac{7h^2}{4}f^{(v)}(x)$

(iii)

	Finite Difference Formula	Leading Order Error
$f''(x)$	$\frac{11f_{i-4}-56f_{i-3}+114f_{i-2}-104f_{i-1}+35f_i}{12h^2}$	$-\frac{5h^3}{6}f^{(v)}(x)$
$f^{(iv)}(x)$	$\frac{f_{i-4}-4f_{i-3}+6f_{i-2}-4f_{i-1}+f_i}{h^4}$	$-2hf^{(v)}(x)$
$f'''(x)-3f'(x)$	$\frac{3f_{i-4}-14f_{i-3}+24f_{i-2}-18f_{i-1}+5f_i}{2h^3}+\frac{-3f_{i-4}+16f_{i-3}-36f_{i-2}+48f_{i-1}-25f_i}{4h}$	$-\frac{7h^2}{4}f^{(v)}(x)$

(iv)

	Finite Difference Formula	Leading Order Error
$f''(x)$	$\frac{2f_{i-1}-4f_i+2f_{i+1}}{h^2}+\frac{f'_{i-1}-f'_{i+1}}{2h}$	$-\frac{h^4}{360}f^{(vi)}(x)$
$f^{(iv)}(x)$	$\frac{-12f_{i-1}+24f_i-12f_{i+1}}{h^4}+\frac{-6f'_{i-1}+6f'_{i+1}}{h^3}$	$+\frac{h^2}{15}f^{(vi)}(x)$
$f'''(x)-3f'(x)$	$\frac{-15f_{i-1}+15f_{i+1}}{2h^3}+\frac{-3f'_{i-1}-24f'_i-3f'_{i+1}}{2h^2}-3f'_i$	$-\frac{h^4}{840}f^{(vii)}(x).$

4. *Use the second order accurate second derivative central difference formula*

$$f''(x) \simeq \frac{f(x+h) - 2f(x) + f(x-h)}{h^2},$$

along with Richardson extrapolation to obtain a fourth and then sixth order accurate second derivative finite difference formula with leading order error. How does this result compare to the results from question 3(a)i?

To obtain a fourth order accurate solution using Richardson Extrapolation, only two second order approximations are necessary. This is because the third order error is not present in the central difference scheme because of symmetries. To do this I chose to do the central difference formulas with h and $\frac{h}{2}$ as the step sizes. Expanding these formulas and keeping their error terms yields the following:

$$\begin{array}{l} \frac{f(x+h)-2f(x)+f(x-h)}{h^2} = f''(x) - \frac{h^2}{12}f^{(iv)}(x) - \frac{h^4}{360}f^{(vi)}(x) - \frac{h^6}{20160}f^{(viii)}(x) - \ldots \quad \text{and} \\ \frac{f(x+\frac{h}{2})-2f(x)+f(x-\frac{h}{2})}{\left(\frac{h}{2}\right)^2} = f''(x) - \frac{h^2}{48}f^{(iv)}(x) - \frac{h^4}{5760}f^{(vi)}(x) - \frac{h^6}{1290240}f^{(viii)}(x) - \ldots \end{array}$$

A linear combination of these two equations can be made such that the second derivative term is retained with a unity coefficient and the second order error term is eliminated. This can be solved for with the following set of equations

$$\begin{bmatrix} 1 & 1 \\ -\frac{h^2}{12} & -\frac{h^2}{48} \end{bmatrix} \begin{bmatrix} F_{[h]} \\ F_{[\frac{h}{2}]} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

which has the solution

$$\begin{bmatrix} F_{[h]} \\ F_{[\frac{h}{2}]} \end{bmatrix} = \begin{bmatrix} -\frac{1}{3} \\ \frac{4}{3} \end{bmatrix}.$$

Notice that the sum of the coefficients for the equations equals one. The leading order error term can be found by including the higher order terms from the Taylor Expansions in the matrix equation

$$\begin{bmatrix} 1 & 1 \\ -\frac{h^2}{12} & -\frac{h^2}{48} \\ -\frac{h^4}{360} & -\frac{h^4}{5760} \end{bmatrix} \begin{bmatrix} -\frac{1}{3} \\ \frac{4}{3} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \frac{h^4}{1440} \end{bmatrix}.$$

Summing the equations, the fourth order second derivative finite difference formula found with Richardson Extrapolation is

$$f''(x) = \frac{-f(x+h) + 16f(x+\frac{h}{2}) - 30f(x) + 16f(x-\frac{h}{2}) - f(x-h)}{3h^2} - \frac{h^4}{1440}f^{(iv)}(x) + \ldots$$

Notice that the coefficients of all the terms sum to zero. This result is the same formula that is found in question 3(a)i when using half step size instead of full step size. To show this, substitute $\hat{h} = \frac{h}{2}$ into the equation which results in

$$f''(x) = \frac{-f(x+2\hat{h}) + 16f(x+\hat{h}) - 30f(x) + 16f(x-\hat{h}) - f(x-2\hat{h})}{12\hat{h}^2} - \frac{\hat{h}^4}{90}f^{(iv)}(x) + \ldots$$

The sixth order accurate solution is found in a very similar fashion, by adding a third central difference equation to allow the elimination of the second and fourth order error terms. For this, I chose to add the central difference formula with $\frac{h}{4}$ as the step size. Expanding this formula and keeping the error terms yields

$$\frac{f(x+\frac{h}{4}) - 2f(x) + f(x-\frac{h}{4})}{\left(\frac{h}{4}\right)^2} = f''(x) - \frac{h^2}{192}f^{(iv)}(x) - \frac{h^4}{92160}f^{(vi)}(x) - \frac{h^6}{82575360}f^{(viii)}(x) - \ldots .$$

This sets up the system of equations

$$\begin{bmatrix} 1 & 1 & 1 \\ -\frac{h^2}{12} & -\frac{h^2}{48} & -\frac{h^2}{192} \\ -\frac{h^4}{360} & -\frac{h^4}{5760} & -\frac{h^4}{92160} \end{bmatrix} \begin{bmatrix} F_{[h]} \\ F_{[\frac{h}{2}]} \\ F_{[\frac{h}{4}]} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix},$$

which has the solution

$$\begin{bmatrix} F_{[h]} \\ F_{[\frac{h}{2}]} \\ F_{[\frac{h}{4}]} \end{bmatrix} = \begin{bmatrix} \frac{1}{45} \\ -\frac{20}{45} \\ \frac{64}{45} \end{bmatrix}.$$

Again, the sum of the coefficients for all of the equations equals one. Adding in the higher order terms the leading error is found to be

$$\begin{bmatrix} 1 & 1 & 1 \\ -\frac{h^2}{12} & -\frac{h^2}{48} & -\frac{h^2}{192} \\ -\frac{h^4}{360} & -\frac{h^4}{5760} & -\frac{h^4}{92160} \\ -\frac{h^6}{20160} & -\frac{h^6}{1290240} & -\frac{h^6}{82575360} \end{bmatrix} \begin{bmatrix} \frac{1}{45} \\ -\frac{20}{45} \\ \frac{64}{45} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ -\frac{h^6}{1290240} \end{bmatrix}.$$

These equations can now be summed to yield the sixth order second derivative finite difference formula

$$f''(x) = \frac{f(x+h)-80f(x+\frac{h}{2})+1024f(x+\frac{h}{4})-1890f(x)+1024f(x-\frac{h}{2})-80f(x+\frac{h}{2})+f(x-h)}{45h^2} + \frac{h^6}{1290240}f^{(iv)}(x) + \dots\ .$$

Again, the coefficients sum to zero. Note that this solution is only unique for this choices of step size. A different choice of step sizes would yield a different solution.

5. *Show the following:*

(a) $\Delta f(x) = \nabla E f(x)$

(b) $\nabla f(x) = \Delta E^{-1} f(x)$

(c) $\nabla \Delta f(x) = \Delta \nabla f(x) = \delta^2 f(x)$

(d) $\Delta^n f(x) = \nabla^n f(x + nh) = \delta^n f\left(x + \frac{nh}{2}\right)$

(e) $\Delta\left(f(x)g(x)\right) = f(x)\Delta g(x) + g(x+h)\Delta f(x)$

(f) $\Delta\left(\frac{f(x)}{g(x)}\right) = \frac{g(x)\Delta f(x) - f(x)\Delta g(x)}{g(x)g(x+h)}$

(a)

$$\begin{array}{rcl} \Delta f(x) & = & \nabla E f(x) \\ & & \nabla\left[f(x+h)\right] \\ & & f\left((x+h)\right) - f\left((x+h)-h\right) \\ & & f(x+h) - f(x) \\ & & \Delta f(x) \end{array}$$

(b)

$$\begin{array}{rcl} \nabla f(x) & = & \Delta E^{-1} f(x) \\ & & \Delta\left[f(x-h)\right] \\ & & f\left((x-h)+h\right) - f\left((x-h)\right) \\ & & f(x) - f(x-h) \\ & & \nabla f(x) \end{array}$$

(c)

$$\begin{array}{rcl} \delta^2 f(x) & = & \delta\delta f(x) \\ & & \delta\left[f(x+\frac{h}{2}) - f(x-\frac{h}{2})\right] \\ & & \delta f(x+\frac{h}{2}) - \delta f(x-\frac{h}{2}) \\ & & \left(f\left((x+\frac{h}{2})+\frac{h}{2}\right) - f\left((x+\frac{h}{2})-\frac{h}{2}\right)\right) - \left(f\left((x-\frac{h}{2})+\frac{h}{2}\right) - f\left((x-\frac{h}{2})-\frac{h}{2}\right)\right) \\ & & f(x+h) - 2f(x) + f(x-h) \end{array}$$

$$\begin{array}{rcl} \nabla\Delta f(x) & = & \nabla\left[f(x+h) - f(x)\right] \\ & & \nabla f(x+h) - \nabla f(x) \\ & & \left(f\left((x+h)\right) - f\left((x+h)-h\right)\right) - \left(f(x) - f(x-h)\right) \\ & & f(x+h) - 2f(x) + f(x-h) \\ & & \delta^2 f(x) \end{array}$$

$$\begin{array}{rcl} \Delta\nabla f(x) & = & \Delta\left[f(x) - f(x-h)\right] \\ & & \Delta f(x) - \Delta f(x-h) \\ & & \left(f(x+h) - f(x)\right) - \left(f\left((x-h)+h\right) - f\left((x-h)\right)\right) \\ & & f(x+h) - 2f(x) + f(x-h) \\ & & \delta^2 f(x) \end{array}$$

(d)

$$\begin{aligned}
\Delta^n f(x) &= \nabla^n f(x+nh) \\
&\textstyle\sum_{i=0}^n = (-1)^i \frac{n!}{i!(n-i)!} f\left((x+nh)-ih\right) \\
&\textstyle\sum_{i=0}^n = (-1)^i \frac{n!}{i!(n-i)!} f\left(x+(n-i)h\right) \\
&\Delta^n f(x)
\end{aligned}$$

$$\begin{aligned}
\Delta^n f(x) &= \delta^n f(x+\tfrac{nh}{2}) \\
&\textstyle\sum_{i=0}^n = (-1)^i \frac{n!}{i!(n-i)!} f\left(\left(x+\frac{nh}{2}\right)+\left(\frac{n}{2}-i\right)h\right) \\
&\textstyle\sum_{i=0}^n = (-1)^i \frac{n!}{i!(n-i)!} f\left(x+(n-i)h\right) \\
&\Delta^n f(x)
\end{aligned}$$

(e)

$$\begin{aligned}
\Delta\left(f(x)g(x)\right) &= f(x)\Delta g(x)+g(x+h)\Delta f(x) \\
&f(x)\left(g(x+h)-g(x)\right)+g(x+h)\left(f(x+h)-f(x)\right) \\
&f(x+h)g(x+h)-f(x)g(x) \\
&\Delta\left(f(x)g(x)\right)
\end{aligned}$$

(f)

$$\begin{aligned}
\Delta\left(\tfrac{f(x)}{g(x)}\right) &= \tfrac{g(x)\Delta f(x)-f(x)\Delta g(x)}{g(x)g(x+h)} \\
&\tfrac{g(x)(f(x+h)-f(x))-f(x)(g(x+h)-g(x))}{g(x)g(x+h)} \\
&\tfrac{g(x)f(x+h)-f(x)g(x+h)}{g(x)g(x+h)} \\
&\tfrac{f(x+h)}{g(x+h)}-\tfrac{f(x)}{g(x)} \\
&\Delta\left(\tfrac{f(x)}{g(x)}\right)
\end{aligned}$$

6. *Integrate following functions of x*

   (a) $\exp(x - \frac{\pi}{4})$,

   (b) $1 - \left|x - \frac{\pi}{4}\right|^{\frac{1}{3}}$,

   (c) $(x - \pi/4)^2 + \frac{3}{4} + \frac{x}{500\left(x-\frac{\pi}{4}\right)^2 + \pi}$,

   on the domain $x \in [0, 1]$. Calculating the actual integrals for each function. Then estimate the integrals using the following quadrature methods:

   i *Trapezoid Rule,*

   ii *Simpson's Rule,*

   iii *3-Point Gauss Quadrature,*

   iv *Adaptive Quadrature.*

   Start with a few points (high target error for the adaptive quadrature) and increase the number of points (decrease target error for the adaptive quadrature) in order to generate a log-log *plot for each function plotting the error against the number of points. Discuss your results.*

   The actual integrals, accurate up to 10^{-18}, are as listed here:

$$
\begin{aligned}
\int_0^1 \exp(x - \tfrac{\pi}{4})dx &= 0.783430199841949948,\\
\int_0^1 1 - \left|x - \tfrac{\pi}{4}\right|^{\frac{1}{3}} dx &= 0.360161072060995680,\\
\int_0^1 (x - \pi/4)^2 + \tfrac{3}{4} + \tfrac{x}{500\left(x-\frac{\pi}{4}\right)^2 + \pi} dx &= 0.965559380738167605.
\end{aligned}
$$

   It is important to include at least this many significant digits (more if you are working with higher than double precision) as the quadrature methods will converge to approximate these answers up to machine precision. If fewer digits are included the error will asymptotically approach the error in what has been omitted from the actual integral.

   These integrals are approximated with the Trapezoidal Rule

$$
I_T \approx h\left(\frac{f_0 + f_N}{2} + \sum_{i=1}^{N-1} f_i\right),
$$

   the Simpson's Rule

$$
I_S \approx \frac{h}{3}\left(f_0 + f_N + 4\sum_{\substack{i=1\\ i=\text{odd}}}^{N-1} f_i + 2\sum_{\substack{i=2\\ i=\text{even}}}^{N-2} f_i\right),
$$

   (which must be applied to an odd set of points), and the 3-point Gauss Quadrature

$$
I_{G_3} \approx \frac{h}{18}\sum_{i=1}^{N-1}\left[5f\left(\frac{x_{i+1}+x_i}{2} - \frac{x_{i+1}-x_i}{2}\sqrt{\frac{3}{5}}\right) + 8f\left(\frac{x_{i+1}+x_i}{2}\right) + 5f\left(\frac{x_{i+1}+x_i}{2} + \frac{x_{i+1}+x_i}{2}\sqrt{\frac{3}{5}}\right)\right],
$$

   where the quadrature is applied piecewise over the domain, three points per segment. This means that the number of points N will be a multiple of three.

   The final approximation is done using the adaptive quadrature method, which checks the approximate error by comparing the quadrature scheme being used over using two grid spacings for each subdomain. This error can then be checked against a specified global tolerance, and if deemed adequate, the quadrature on the fine mesh can be kept for that domain. If the error is too large the fine mesh

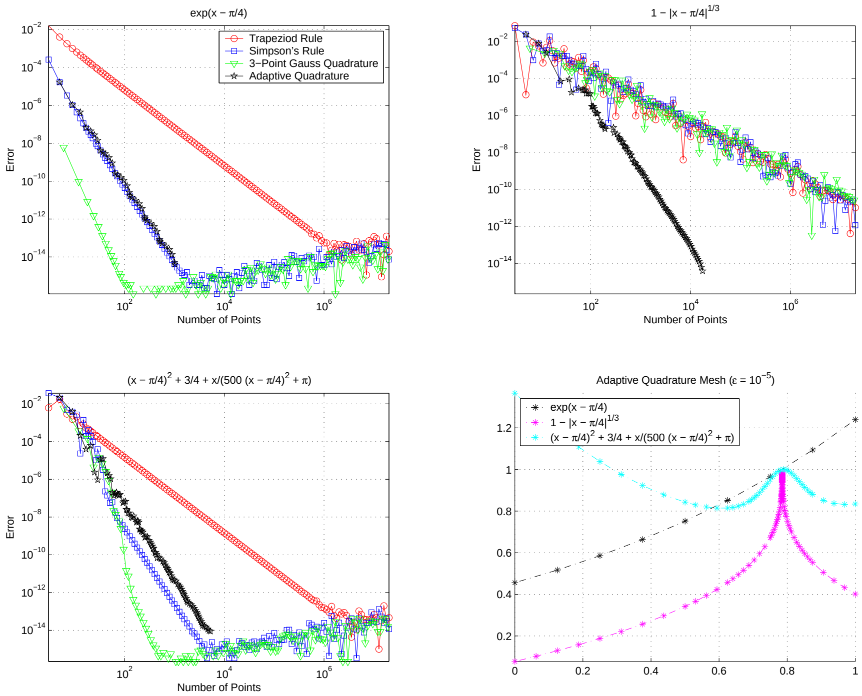

Figure 7: Quadrature Error and Mesh

quadrature can be compared to a quadrature on a still finer mesh iteratively until the error meets the tolerance demanded. For the adaptive quadrature, any of the quadrature methods can be used; I chose to follow Simpson's Rule, which is outlined in the course notes.

For each of the first three methods, I increased the number of points, and recorded the error by taking the difference between the quadrature and the actual integral. For the adaptive method, I decreased the target error, then recorded how may points were in the adaptive grid and the final error. These errors are plotted against the number of point in figure 7. The linear regression of the asymptotic regime for each of the methods is listed in the table below.

	$\exp(x - \frac{\pi}{4})$	$1 - \left\|x - \frac{\pi}{4}\right\|^{\frac{1}{3}}$	$(x - \pi/4)^2 + \frac{3}{4} + \frac{x}{500\left(x-\frac{\pi}{4}\right)^2+\pi}$
Trapezoid Rule	$-2.65N^{-2.01}$	$-2.57N^{-1.33}$	$-1.89N^{-2.00}$
Simpson's Rule	$-5.06N^{-4.06}$	$-2.36N^{-1.34}$	$-1.28N^{-4.02}$
3-Point Gauss Quadrature	$-6.61N^{-6.32}$	$-2.27N^{-1.38}$	$1.95N^{-6.06}$
Adaptive Quadrature	$-4.60N^{-4.06}$	$7.48N^{-4.08}$	$1.80N^{-4.04}$

Notice that the exponential (a) and the fraction (c) functions display the anticipated convergence rate for each scheme once they have entered the asymptotic regime. The adaptive quadrature follows the convergence rate as its base scheme the Simpson's rule. The fraction function takes a larger number of points to enter the asymptotic regime because of the areas with high derivatives.

The absolute value cube root (b) function does not display the anticipated convergence rate, which means that it does not enter the asymptotic regime for up to 2×10^7 points. This is due to the cusp in the function which has discontinuous derivatives. It is not shown here, but is interesting to note that if the domain were split in two at the cusp and an integral was evaluated on each subdomain, the expected convergence rates would still not be found on up to 2×10^7 points. The adaptive quadrature on this function, however, does converge at the expected rate for Simpson's Rule. The reason for this is apparent when the mesh is observed. Figure 7 shows an example of the adaptive quadrature mesh for each function when the target error is 10^{-5}. Notice how the points are clustered in the areas with large derivatives and more dispersed in other areas. This clustering of points around the cusp is what allows the adaptive quadrature to converge quickly on the absolute value cube root function.

Notice also that the error has a minimum value $O(10^{-16})$. This is because of machine precision, and while it can be improved by using higher than double precision to represent values, therefore reducing the round-off error, it cannot be eliminated on a discrete counting machine like a computer.