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MATH 561 Numerical Analysis I
Homework 3

1. (a) Use the central quotient approximation $f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$ to obtain an approximation of $\frac{\partial^2}{\partial x \partial y} u(x,y)$, for a function u of two variables.

$$\begin{aligned}
\frac{\partial^2}{\partial x \partial y} u(x,y) &= \frac{\partial}{\partial x}\left(\frac{\partial}{\partial y} u(x,y)\right) \\
&\approx \frac{\partial}{\partial x}\left(\frac{u(x,y+h) - u(x,y-h)}{2h}\right) \\
&= \frac{1}{2h}\left(\frac{\partial}{\partial x} u(x,y+h) - \frac{\partial}{\partial x} u(x,y-h)\right) \\
&\approx \frac{1}{2h}\left(\frac{u(x+h,y+h) - u(x-h,y+h)}{2h} - \frac{u(x+h,y-h) - u(x-h,y-h)}{2h}\right) \\
&= \frac{u(x+h,y+h) - u(x-h,y+h) - u(x+h,y-h) + u(x-h,y-h)}{4h^2}
\end{aligned}$$

(b) The fourth order Taylor expansion of $u(v,w)$ approximated at (x,y) is

$$\begin{aligned}
u(v,w) = u(x,y) &+ (v-x)\frac{\partial}{\partial x}(u(x,y)) + (w-y)\frac{\partial}{\partial y}(u(x,y)) + \frac{(v-x)^2}{2}\frac{\partial^2}{\partial x^2}(u(x,y)) \\
&+ (v-x)(w-y)\frac{\partial^2}{\partial x \partial y}(u(x,y)) + \frac{(w-y)^2}{2}\frac{\partial^2}{\partial y^2}(u(x,y)) + \frac{(v-x)^3}{3!}\frac{\partial^3}{\partial x^3}(u(x,y)) \\
&+ \frac{(v-x)^2(w-y)}{2!}\frac{\partial^3}{\partial x^2 \partial y}(u(x,y)) + \frac{(v-x)(w-y)^2}{2!}\frac{\partial^3}{\partial x \partial y^2}(u(x,y)) \\
&+ \frac{(w-y)^3}{3!}\frac{\partial^3}{\partial y^3}(u(x,y)) + \frac{(v-x)^4}{4!}\frac{\partial^4}{\partial x^4}(u(x,y)) + \frac{(v-x)^3(w-y)}{3!}\frac{\partial^4}{\partial x^3 \partial y}(u(x,y)) \\
&+ \frac{(v-x)^2(w-y)^2}{2!2!}\frac{\partial^4}{\partial x^2 \partial y^2}(u(x,y)) + \frac{(v-x)(w-y)^3}{3!}\frac{\partial^4}{\partial x \partial y^3}(u(x,y)) \\
&+ \frac{(w-y)^4}{4!}\frac{\partial^4}{\partial y^4}(u(x,y))
\end{aligned}$$

Taking the fourth order Taylor expansion of the terms found in part (a)

$$\begin{aligned}
&\frac{u(x+h,y+h) - u(x-h,y+h) - u(x+h,y-h) + u(x-h,y-h)}{4h^2} \\
&\approx \frac{1}{4h^2}(u(x,y) + h\frac{\partial}{\partial x}(u(x,y)) + h\frac{\partial}{\partial y}(u(x,y)) + \frac{h^2}{2}\frac{\partial^2}{\partial x^2}(u(x,y))
\end{aligned}$$

$$
\begin{aligned}
&+ h^2 \frac{\partial^2}{\partial x \partial y}(u(x,y)) + \frac{h^2}{2}\frac{\partial^2}{\partial y^2}(u(x,y)) + \frac{h^3}{3!}\frac{\partial^3}{\partial x^3}(u(x,y)) \\
&+ \frac{h^3}{2!}\frac{\partial^3}{\partial x^2 \partial y}(u(x,y)) + \frac{h^3}{2!}\frac{\partial^3}{\partial x \partial y^2}(u(x,y)) \\
&+ \frac{h^3}{3!}\frac{\partial^3}{\partial y^3}(u(x,y)) + \frac{h^4}{4!}\frac{\partial^4}{\partial x^4}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x^3 \partial y}(u(x,y)) \\
&+ \frac{h^4}{2!2!}\frac{\partial^4}{\partial x^2 \partial y^2}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x \partial y^3}(u(x,y)) \\
&+ \frac{h^4}{4!}\frac{\partial^4}{\partial y^4}(u(x,y)) - u(x,y) + h\frac{\partial}{\partial x}(u(x,y)) - h\frac{\partial}{\partial y}(u(x,y)) - \frac{h^2}{2}\frac{\partial^2}{\partial x^2}(u(x,y)) \\
&+ h^2 \frac{\partial^2}{\partial x \partial y}(u(x,y)) - \frac{h^2}{2}\frac{\partial^2}{\partial y^2}(u(x,y)) + \frac{h^3}{3!}\frac{\partial^3}{\partial x^3}(u(x,y)) \\
&- \frac{h^3}{2!}\frac{\partial^3}{\partial x^2 \partial y}(u(x,y)) + \frac{h^3}{2!}\frac{\partial^3}{\partial x \partial y^2}(u(x,y)) \\
&- \frac{h^3}{3!}\frac{\partial^3}{\partial y^3}(u(x,y)) - \frac{h^4}{4!}\frac{\partial^4}{\partial x^4}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x^3 \partial y}(u(x,y)) \\
&- \frac{h^4}{2!2!}\frac{\partial^4}{\partial x^2 \partial y^2}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x \partial y^3}(u(x,y)) \\
&- \frac{h^4}{4!}\frac{\partial^4}{\partial y^4}(u(x,y)) - u(x,y) - h\frac{\partial}{\partial x}(u(x,y)) + h\frac{\partial}{\partial y}(u(x,y)) - \frac{h^2}{2}\frac{\partial^2}{\partial x^2}(u(x,y)) \\
&+ h^2 \frac{\partial^2}{\partial x \partial y}(u(x,y)) - \frac{h^2}{2}\frac{\partial^2}{\partial y^2}(u(x,y)) - \frac{h^3}{3!}\frac{\partial^3}{\partial x^3}(u(x,y)) \\
&+ \frac{h^3}{2!}\frac{\partial^3}{\partial x^2 \partial y}(u(x,y)) - \frac{h^3}{2!}\frac{\partial^3}{\partial x \partial y^2}(u(x,y)) \\
&+ \frac{h^3}{3!}\frac{\partial^3}{\partial y^3}(u(x,y)) - \frac{h^4}{4!}\frac{\partial^4}{\partial x^4}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x^3 \partial y}(u(x,y)) \\
&- \frac{h^4}{2!2!}\frac{\partial^4}{\partial x^2 \partial y^2}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x \partial y^3}(u(x,y)) \\
&- \frac{h^4}{4!}\frac{\partial^4}{\partial y^4}(u(x,y)) + u(x,y) - h\frac{\partial}{\partial x}(u(x,y)) - h\frac{\partial}{\partial y}(u(x,y)) + \frac{h^2}{2}\frac{\partial^2}{\partial x^2}(u(x,y)) \\
&+ h^2 \frac{\partial^2}{\partial x \partial y}(u(x,y)) + \frac{h^2}{2}\frac{\partial^2}{\partial y^2}(u(x,y)) - \frac{h^3}{3!}\frac{\partial^3}{\partial x^3}(u(x,y)) \\
&- \frac{h^3}{2!}\frac{\partial^3}{\partial x^2 \partial y}(u(x,y)) - \frac{h^3}{2!}\frac{\partial^3}{\partial x \partial y^2}(u(x,y)) \\
&- \frac{h^3}{3!}\frac{\partial^3}{\partial y^3}(u(x,y)) + \frac{h^4}{4!}\frac{\partial^4}{\partial x^4}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x^3 \partial y}(u(x,y))
\end{aligned}
$$

$$
\begin{aligned}
&+ \frac{h^4}{2!2!}\frac{\partial^4}{\partial x^2 \partial y^2}(u(x,y)) + \frac{h^4}{3!}\frac{\partial^4}{\partial x \partial y^3}(u(x,y)) \\
&+ \frac{h^4}{4!}\frac{\partial^4}{\partial y^4}(u(x,y))) \\
&= \frac{1}{4h^2}\left(\frac{2h^4}{3}\frac{\partial^4}{\partial x^3 \partial y}(u(x,y)) + 4h^2\frac{\partial^2}{\partial x \partial y}(u(x,y)) + \frac{2h^4}{3}\frac{\partial^4}{\partial x \partial y^3}(u(x,y))\right) \\
&= \frac{\partial^2}{\partial x \partial y}(u(x,y)) + \frac{h^2}{6}\left(\frac{\partial^4}{\partial x^3 \partial y}(u(x,y)) + \frac{\partial^4}{\partial x \partial y^3}(u(x,y))\right) \\
&= \frac{\partial^2}{\partial x \partial y}(u(x,y)) + O(h^2)
\end{aligned}
$$

2. Let s be a function defined by

$$
s(x) = \begin{cases} (x+1)^3 & -1 \le x \le 0 \\ (1-x)^3 & 0 \le x \le 1 \end{cases}
$$

(a) With Δ denoting the subdivision of $[-1,1]$ into $[-1,0]$ and $[0,1]$, to what class $S_m^k(\Delta)$ does the spline s belong to?

Since each piece of s is degree 3, the degree of s is $m = 3$. Let $s_1(x) = (x+1)^3$ and let $s_2(x) = (1-x)^3$. Then s is continuous because $s_1(0) = (0+1)^3 = 1 = (1-0)^3 = s_2(0)$. Also $s_1'(0) = 3(0+1)^2 = 3$ and $s_2'(0) = -3(1-0)^2 = -3$, therefore the first derivative of s is not continuous. So s belongs to smoothness class $k = 0$.

(b) Estimate the error of the composite trapezoidal rule applied to $\int_{-1}^{1} s(x)\,\mathrm{d}x$, when $[-1,1]$ is divided into n subintervals of equal length $h = 2/n$ and n is even.

Since n is even the composite trapezoidal rule can be broken into two subintervals, $[-1,0]$ and $[0,1]$. The total error is then the sum of the errors on the two parts.

$$
\begin{aligned}
E &= -\frac{1}{12}h^2 s_1''(\xi_1) - \frac{1}{12}h^2 s_2''(\xi_2) \\
&= -\frac{1}{12}h^2(s_1''(\xi_1) + s_2''(\xi_2))
\end{aligned}
$$

This is for $-1 < \xi_1 < 0$ and $0 < \xi_2 < 1$. The second derivatives of each piece are $s_1''(x) = 6(x+1)$ and $s_2''(x) = 6(1-x)$. These are both positive, so the estimate will be larger than the actual integral, so the error will be negative as can be seen in the error formula. We can find an upper bound for the error, by noting that the second derivatives are bounded, that is $s_1''(\xi_1) < 6$ and $s_2''(\xi_2) < 6$. Therefore $(s_1''(\xi_1) + s_2''(\xi_2)) < 12$. This implies that the error can be bounded by $-h^2$, that is

$$
-h^2 > E > 0
$$

(c) What is the error of the composite Simpson's rule applied to $\int_{-1}^{1} s(x)\,\mathrm{d}x$, with the same subdivision of $[-1, 1]$ as in (b)?

Simpson's rule has a degree of exactness equal to 3. Simpson's rule is applied to every two intervals, since n is even Simpson's rule can be applied to s over the subdivision Δ.

Since n is even either $n = 4m$ or $n = 4m + 2$ for some positive integer m. If $n = 4m$ for some positive integer m, that is n is a multiple of 4, then $\int_{-1}^{1} s(x)\,\mathrm{d}x$ can be approximated by applying Simpson's rule to $\int_{-1}^{0} s(x)\,\mathrm{d}x$ and $\int_{0}^{1} s(x)\,\mathrm{d}x$ separately and summing. This can be done because there $n/2 = 2m$ intervals on $[-1, 0]$ and $[0, 1]$. Each of these integrals can be evaluated exactly because Simpson's rule has degree of exactness equal to 3. Therefore the total error is 0.

If $n = 4m+2$ for some positive integer m, then $\int_{-1}^{1} s(x)\,\mathrm{d}x$ can be approximated by applying Simpson's rule to $\int_{-1}^{-h} s(x)\,\mathrm{d}x$, $\int_{-h}^{h} s(x)\,\mathrm{d}x$, and $\int_{h}^{1} s(x)\,\mathrm{d}x$ separately and summing. In this situation each interval $[-1, 0]$ and $[0, 1]$ has an odd number of subintervals, so Simpson's rule must be applied across the interval $[-h, h]$. Simpson's rule evaluates $\int_{-1}^{-h} s(x)\,\mathrm{d}x$ and $\int_{h}^{1} s(x)\,\mathrm{d}x$ exactly because $s(x)$ is a degree 3 polynomial on these intervals. Therefore the error from Simpson's rule comes when approximating the integral $\int_{-h}^{h} s(x)\,\mathrm{d}x$. The error can be found as follows.

$$
\begin{aligned}
E &= \int_{-h}^{h} s(x)\,\mathrm{d}x - \frac{h}{3}(s(-h) + 4s(0) + s(h)) \\
&= \int_{-h}^{0} (x+1)^3\,\mathrm{d}x + \int_{0}^{h} (1-x)^3\,\mathrm{d}x - \frac{h}{3}\Big((1-h)^3 + 4 + (1-h)^3\Big) \\
&= \frac{1}{4}(x+1)^4\Big|_{x=-h}^{0} + -\frac{1}{4}(1-x)^4\Big|_{x=0}^{h} - \frac{h}{3}\Big(2(1-h)^3 + 4\Big) \\
&= \frac{1}{4}\Big(1 - (1-h)^4\Big) - \frac{1}{4}\Big((1-h)^4 - 1\Big) - \frac{h}{3}\Big(2(1-h)^3 + 4\Big) \\
&= \frac{1}{2} - \frac{1}{2}(1-h)^4 - \frac{4h}{3} - \frac{2h}{3}(1-h)^3 \\
&= (1-h)^3\left(-\frac{1}{2}(1-h) - \frac{2h}{3}\right) - \frac{4h}{3} + \frac{1}{2} \\
&= (1-h)^3\left(-\frac{h}{6} - \frac{1}{2}\right) - \frac{4h}{3} + \frac{1}{2}
\end{aligned}
$$

This is also the total error.

(d) What is the error resulting from applying the 2-point Gauss-Legendre rule to $\int_{-1}^{0} s(x)\,\mathrm{d}x$ and $\int_{0}^{1} s(x)\,\mathrm{d}x$ separately and summing?

The 2-point Gauss-Legendre rule has degree of exactness equal to 3. So on each of these intervals the $s(x)$ is a degree 3 polynomial, therefore the error on each of these intervals will be zero. So the total error is zero.

3. (a) Determine by Hermite interplation the quadractic polynomial p interpolating f at $x = 0$ and $x = 1$ and f' at $x = 0$. Also express the errors in terms of an appropriate derivative.

x	$f(x)$		
0	$f(0)$		
0	$f(0)$	$f'(0)$	
1	$f(1)$	$f(1) - f(0)$	$f(1) - f(0) - f'(0)$

Therefore $p(x) = f(0) + f'(0)x + (f(1) - f(0) - f'(0))x^2 + x^2(x-1)\frac{f'''(\xi)}{6}$, where the error is $x^2(x-1)\frac{f'''(\xi)}{6}$ for some $0 < \xi < 1$

(b) Using the interpolation polynomial found in (a), $\int_0^1 f(x)\,\mathrm{d}x \approx \int_0^1 p(x)\,\mathrm{d}x$.

$$\begin{aligned}
\int_0^1 p(x)\,\mathrm{d}x &= \int_0^1 f(0) + f'(0)x + (f(1) - f(0) - f'(0))x^2\,\mathrm{d}x \\
&= f(0)x + \frac{1}{2}f'(0)x^2 + \frac{1}{3}(f(1) - f(0) - f'(0))x^3\Big|_{x=0}^{1} \\
&= f(0) + \frac{1}{2}f'(0) + \frac{1}{3}(f(1) - f(0) - f'(0)) \\
&= \frac{2}{3}f(0) - \frac{1}{3}f(1) + \frac{1}{6}f'(0)
\end{aligned}$$

Therefore

$$\int_0^1 f(x)\,\mathrm{d}x \approx \frac{2}{3}f(0) - \frac{1}{3}f(1) + \frac{1}{6}f'(0)$$

This can be expressed as the integration formula $\int_0^1 f(x)\,\mathrm{d}x \approx a_0 f(0) + a_1 f(1) + b_0 f'(0)$, where $a_0 = \frac{2}{3}$, $a_1 = -\frac{1}{3}$, and $b_0 = \frac{1}{6}$.

The error term for this quadrature formula can be found by integrating, the error of the polynomial.

$$E(f) = \int_0^1 x^2(x-1)\frac{f'''(\xi)}{6}\,\mathrm{d}x$$

Since $x^2(x-1)$ does not change sign over the interval $(0, 1)$

$$\begin{aligned}
&= \frac{f'''(\xi)}{6}\int_0^1 x^2(x-1)\,\mathrm{d}x \\
&= \frac{f'''(\xi)}{6}\int_0^1 x^3 - x^2\,\mathrm{d}x
\end{aligned}$$

$$
\begin{aligned}
&= \frac{f'''(\xi)}{6}\left(\frac{1}{4}x^4 - \frac{1}{3}x^3\right)\Big|_{x=0}^{1} \\
&= \frac{f'''(\xi)}{6}\left(\frac{1}{4} - \frac{1}{3}\right) \\
&= -\frac{f'''(\xi)}{72}
\end{aligned}
$$

(c) Transform the result of (b) to obtain an integration rule, with remainder, for $\int_c^{c+h} y(t)\,\mathrm{d}t$.

This can be accomplished by linearly mapping the interval $(0,1)$ to $(c, c+h)$, which is equivalent to a change of variables $t \to c + xh$. Thus $f(x) = y(c + xh)$.

$$
\begin{aligned}
\int_c^{c+h} y(t)\,\mathrm{d}t &= \int_0^1 y(c + xh)\,\mathrm{d}x \\
&= \frac{2}{3}y(c) - \frac{1}{3}y(c+h) + \frac{h}{6}y'(c) - \frac{h^3}{72}y'''(c + \xi h)
\end{aligned}
$$

Where $0 < \xi < 1$

4. (a) Construct the quadractic (monic) polynomial $\pi_2(t; w)$ orthogonal on $(0, \infty)$ with respect to the weight function $w(t) = e^{-t}$.

The quadractic monic orthogonal polynomial will be in the form, $\pi_2(t; w) = t^2 + p_1 t + p_2$. Since this polynomial is orthogonal to any polynomials of degree 1 or less with respect to the weight $w(t)$ the following two conditions can be imposed, $\int_0^\infty \pi_2(t) f(t) w(t)\,\mathrm{d}t = 0$ for $f(t) = 1$ and $f(t) = t$. These two conditions allow for p_1 and p_2 to be uniquely determined.

$$
\begin{aligned}
0 &= \int_0^\infty \pi_2(t) w(t)\,\mathrm{d}t \\
&= \int_0^\infty \Big(t^2 + p_1 t + p_2\Big) e^{-t}\,\mathrm{d}t \\
&= \int_0^\infty t^2 e^{-t} + p_1 t e^{-t} + p_2 e^{-t}\,\mathrm{d}t
\end{aligned}
$$

Using the fact that $\int_0^\infty t^m e^{-t}\,\mathrm{d}t = m!$

$$
\begin{aligned}
0 &= 2 + p_1 + p_2 \\
0 &= \int_0^\infty t\pi_2(t) w(t)\,\mathrm{d}t \\
&= \int_0^\infty \Big(t^3 + p_1 t^2 + p_2 t\Big) e^{-t}\,\mathrm{d}t
\end{aligned}
$$

$$
\begin{aligned}
&= \int_0^\infty t^3 e^{-t} + p_1 t^2 e^{-t} + p_2 t e^{-t} \, \mathrm{d}t \\
0 &= 6 + 2p_1 + p_2
\end{aligned}
$$

This system of two equations can now be solved for p_1 and p_2.

$$
\begin{aligned}
0 &= 2 + p_1 + p_2 \\
p_1 &= -p_2 - 2 \\
0 &= 6 + 2p_1 + p_2 \\
0 &= 6 - 2p_2 - 4 + p_2 \\
p_2 &= 2 \\
p_1 &= -2 - 2 = -4
\end{aligned}
$$

Therefore the orthogonal quadractic polynomial is $\pi_2(t; w) = t^2 - 4t + 2$

(b) Obtain the two point Gauss-Laguerre quadrature formula.

$$
\int_0^\infty f(t) e^{-t} \, \mathrm{d}t = w_1 f(t_1) + w_2 f(t_2) + E_2(f)
$$

The values of t_1 and t_2 are the zeros of the orthogonal

$$
\begin{aligned}
t &= \frac{4 \pm \sqrt{16 - 4 \cdot 2}}{2} \\
&= \frac{4 \pm 2\sqrt{2}}{2} \\
&= 2 \pm \sqrt{2}
\end{aligned}
$$

Therefore $t_1 = 2 - \sqrt{2}$ and $t_2 = 2 + \sqrt{2}$.

We know that this quadrature formula must be exact for polynomials of degree 1 or less. This gives us two conditions with which to find w_1 and w_2. That is the quadrature formula must be exact for $f(t) = 1$ and $f(t) = t$

$$
\begin{aligned}
\int_0^\infty e^{-t} \, \mathrm{d}t &= w_1 + w_2 \\
1 &= w_1 + w_2 \\
\int_0^\infty t e^{-t} \, \mathrm{d}t &= w_1(2 - \sqrt{2}) + w_2(2 + \sqrt{2}) \\
1 &= w_1(2 - \sqrt{2}) + w_2(2 + \sqrt{2})
\end{aligned}
$$

Now w_1 and w_2 can be found by solving this system of linear equations.

$$
1 = w_1 + w_2
$$

$$
\begin{aligned}
w_1 &= 1 - w_2 \\
1 &= w_1(2-\sqrt{2}) + w_2(2+\sqrt{2}) \\
1 &= (1-w_2)(2-\sqrt{2}) + w_2(2+\sqrt{2}) \\
1 &= 2 - \sqrt{2} + 2\sqrt{2}w_2 \\
w_2 &= \frac{\sqrt{2}-1}{2\sqrt{2}} \\
w_2 &= \frac{2-\sqrt{2}}{4} \\
w_1 &= \frac{2+\sqrt{2}}{4}
\end{aligned}
$$

Also the error term $E_2(f)$ is given by

$$
\begin{aligned}
E_2(f) &= \frac{f^{(4)}(\xi)}{4!}\int_0^\infty \pi_2(t)^2 e^{-t}\,\mathrm{d}t \\
&= \frac{f^{(4)}(\xi)}{4!}\int_0^\infty \Big(t^2-4t+2\Big)^2 e^{-t}\,\mathrm{d}t \\
&= \frac{f^{(4)}(\xi)}{4!}\int_0^\infty \Big(t^4-8t^3+20t^2-16t+4\Big) e^{-t}\,\mathrm{d}t \\
&= \frac{f^{(4)}(\xi)}{4!}(4! - 8\cdot 3! - 20\cdot 2 - 16 + 4) \\
&= \frac{f^{(4)}(\xi)}{24}(24 - 48 + 40 - 16 + 4) \\
&= \frac{f^{(4)}(\xi)}{24}(4) \\
&= \frac{1}{6}f^{(4)}(\xi)
\end{aligned}
$$

for $0 < \xi < \infty$

Therefore the Gauss-Laguerre quadrature formula is

$$
\int_0^\infty f(t)e^{-t}\,\mathrm{d}t = \frac{2+\sqrt{2}}{4}f(2-\sqrt{2}) + \frac{2-\sqrt{2}}{4}f(2+\sqrt{2}) + \frac{1}{6}f^{(4)}(\xi)
$$

(c) Apply the formula in (b) to approximate $I = \int_0^\infty \frac{e^{-t}}{t+1}\,\mathrm{d}t$. Use the remainder term $E_2(f)$ to estimate the error, and compare your estimate with the true error (use I = 0.596347361). Knowing the true error, identify the unknown quantity $\xi > 0$ contained in the error term $E_2(t)$.

Using the quadrature formula

$$
\begin{aligned}
I &= \int_0^\infty f(t)e^{-t}\,\mathrm{d}t \\
&\approx \frac{2+\sqrt{2}}{4} f(2-\sqrt{2}) + \frac{2-\sqrt{2}}{4} f(2+\sqrt{2}) \\
&= \frac{2+\sqrt{2}}{4} \frac{1}{3-\sqrt{2}} + \frac{2-\sqrt{2}}{4} \frac{1}{3+\sqrt{2}} \\
&\approx 0.571428571
\end{aligned}
$$

The error can be estimated by examining $E_2(f)$.

$$
\begin{aligned}
E_2(f) &= \frac{1}{6} f^{(4)}(\xi) \\
f^{(4)}(\xi) &= \frac{24}{(1+\xi)^5} \\
E_2(f) &= \frac{4}{(1+\xi)^5} \\
E_2(f) &< 4
\end{aligned}
$$

The true error is $E_2(f) = 0.596347361 - 0.571428571 = .0249188$. Thus the quantity $\xi > 0$ can be identified as follows

$$
\begin{aligned}
.0249188 &= \frac{4}{(1+\xi)^5} \\
(1+\xi)^5 &= \frac{4}{.0249188} \\
1+\xi &= \left(\frac{4}{.0249188}\right)^{1/5} \\
\xi &= \left(\frac{4}{.0249188}\right)^{1/5} - 1 \\
\xi &\approx 1.761255600
\end{aligned}
$$

5. Consider a quadrature formula of the type

$$\int_0^\infty e^{-x} f(x)\,\mathrm{d}x = af(0) + bf(c) + E(f)$$

(a) Find a, b, and c such that the formula has degree of exactness $d = 2$. Can you identify the formula so obtained?

If the degree of exactness is to be equal to $d = 2$, then the quadrature formula must be exact for $f(x) = 1$, $f(x) = x$, and $f(x) = x^2$.

$$\int_0^\infty e^{-x}\,\mathrm{d}x = a + b$$

$$
\begin{aligned}
1 &= a + b \\
\int_0^\infty x e^{-x}\,\mathrm{d}x &= bc \\
1 &= a + bc \\
\int_0^\infty x^2 e^{-x}\,\mathrm{d}x &= bc^2 \\
2 &= a + bc^2
\end{aligned}
$$

These three equations can now be solved for a, b, and c.

$$
\begin{aligned}
bc &= 1 \\
b &= \frac{1}{c} \\
bc^2 &= 2 \\
\frac{c^2}{c} &= 2 \\
c &= 2 \\
b &= \frac{1}{2} \\
a &= \frac{1}{2}
\end{aligned}
$$

Therefore the quadrature rule will be

$$
\int_0^\infty e^{-x} f(x)\,\mathrm{d}x \approx \frac{1}{2}(f(0) + f(2))
$$

(b) Let $p_2(x) = p_2(f; 0, 2, 2; x)$ be the Hermite interpolation polynomial at the point $x = 0$ and at the double point $x = 2$. Determine $\int_0^\infty p_2(x)e^{-x}\,\mathrm{d}x$ and compare with results in (a).

First we must find the Hermite interpolation polynomial.

x	$f(x)$		
0	$f(0)$		
2	$f(2)$	$(f(2) - f(0))/2$	
2	$f(2)$	$f'(2)$	$([0, 2]f - f'(2))/2$

Thus

$$
p_2(x) = f(0) + \frac{f(2) - f(0)}{2}x + \frac{\frac{f(2)-f(0)}{2} - f'(2)}{2}x(x-2)
$$

$$= f(0) + \left(\frac{f(2) - f(0)}{2} - \frac{f(2) - f(0)}{2} + f'(2)\right)x + \frac{\frac{f(2)-f(0)}{2} - f'(2)}{2}x^2$$

$$= f(0) + f'(2)x + \frac{\frac{f(2)-f(0)}{2} - f'(2)}{2}x^2$$

This interpolation polynomial can be integrated to form a new quadrature formula.

$$\begin{aligned}
\int_0^\infty p_2(x)e^{-x}\,\mathrm{d}x &= \int_0^\infty \left(f(0) + f'(2)x + \frac{\frac{f(2)-f(0)}{2} - f'(2)}{2}x^2\right)e^{-x}\,\mathrm{d}x \\
&= f(0) + f'(2) + \frac{f(2) - f(0)}{2} - f'(2) \\
&= f(0) + \frac{f(2) - f(0)}{2} \\
&= \frac{1}{2}(f(0) + f(2))
\end{aligned}$$

This is the same quadrature formula as found in part (a).

(c) Obtain the remainder $E(f)$ in the form $E(f) = \mathit{const} \cdot f'''(\xi)$, for $\xi > 0$.

The error of the interpolating polynomial $p_2(x)$ can be expressed as $x(x-2)^2\frac{f'''(\xi)}{6}$, for some $\xi > 0$. Integrating this expression, will result in the error for the quadrature formula, since the error of the quadrature is directly related to the error of the interpolation polynomial.

$$E(f) = \int_0^\infty x(x-2)^2\frac{f'''(\xi)}{6}e^{-x}\,\mathrm{d}x$$

Since $x(x-2)^2e^{-x}$ does not change signs over $(0, \infty)$, the Mean Value Theorem for integrals can be applied.

$$\begin{aligned}
&= \frac{f'''(\xi)}{6}\int_0^\infty x(x-2)^2e^{-x}\,\mathrm{d}x \\
&= \frac{f'''(\xi)}{6}\int_0^\infty \left(x^3 - 4x^2 + 4x\right)e^{-x}\,\mathrm{d}x \\
&= \frac{f'''(\xi)}{6}(6 - 8 + 4) \\
&= \frac{f'''(\xi)}{6}(2) \\
&= \frac{f'''(\xi)}{3}
\end{aligned}$$

6. (a) The first column of the Romberg array is the basic composite trapezoidal rule with a shrinking subinterval h. Let $h_k = (b-a)/2^k$ and let T_{h_k} be composite trapezoidal rule with subdivion of h_k, that is

$$T_{h_k} = h_k \left(\frac{1}{2} f(a) + \sum_{r=1}^{2^k-1} (f(a+rh_k)) + \frac{1}{2} f(b) \right)$$

Alse let M_{h_k} be the midpoint rule with subdivision of h_k, that is

$$M_{h_k} = h_k \sum_{r=1}^{2^k} \left(f(a + (r - \frac{1}{2})h_k) \right)$$

Obviously for $k = 0$, $h_k = (b-a)$. Then

$$\begin{aligned} T_{h_0} &= (b-a)\left(\frac{1}{2} f(a) + \sum_{r=1}^{0} (f(a+rh_k)) + \frac{1}{2} f(b) \right) \\ &= (b-a)\left(\frac{1}{2} f(a) + \frac{1}{2} f(b) \right) \\ &= \frac{(b-a)}{2}(f(a)+f(b)) \end{aligned}$$

Thus the bases condition for the recursive definition is valid.
Now consider $T_{k+1,0}$

$$T_{h_{k+1}} = h_{k+1} \left(\frac{1}{2} f(a) + \sum_{r=1}^{2^{k+1}-1} (f(a+rh_{k+1})) + \frac{1}{2} f(b) \right)$$

Note that $h_{k+1} = \frac{1}{2} h_k$

$$= \frac{1}{2} h_k \left(\frac{1}{2} f(a) + \sum_{r=1}^{2^{k+1}-1} \left(f(a + \frac{1}{2} r h_k) \right) + \frac{1}{2} f(b) \right)$$

Also note that r is either even or odd. If r is even then $r = 2n$ for $1 \leq n \leq 2^k - 1$. If r is odd then $r = 2m-1$, for $1 \leq m \leq 2^k$.

$$\begin{aligned} &= \frac{1}{2} h_k \left(\frac{1}{2} f(a) + \sum_{n=1}^{2^k-1} (f(a+nh_k)) + \sum_{m=1}^{2^k} \left(f(a + (m - \frac{1}{2})h_k) \right) + \frac{1}{2} f(b) \right) \\ &= \frac{1}{2} \left(h_k \left(\frac{1}{2} f(a) + \sum_{n=1}^{2^k-1} (f(a+nh_k)) + \frac{1}{2} f(b) \right) + h_k \sum_{m=1}^{2^k} \left(f(a + (m - \frac{1}{2})h_k) \right) \right) \\ &= \frac{1}{2}(T_{k,0} + M_{h_k}) \end{aligned}$$

This verifies the recursive relation.

(b) Code for creating Rnamber array.

```
function [T] = rombergIntegration(a, b, n, f)
    p = inputParser;
    p.addRequired('a', @isnumeric);
    p.addRequired('b', @isnumeric);
    p.addRequired('n', @Utils.isPositiveInteger);
    p.addRequired('f', @Utils.isFunctionHandle);
    p.parse(a, b, n, f);

    T = zeros(n);

    T(1,1) = trapRule(a, b, 0, f);
    % iterate down rows
    for i = 2:n
        T(i,1) = 1/2 * (trapRule(a, b, i-1, f) + midPointRule(a, ...
            b, i-1, f));
        % iterate down columns to diagonal
        for j = 2:i
            T(i,j) = T(i,j-1) + (T(i,j-1) - T(i-1, j-1))/(4^i - 1);
        end
    end
end

function t = trapRule(a, b, k, f)
    hk = computeHK(a, b, k);
    r = 1:(2^k-1);
    functionValues = arrayfun(f, a + r * hk);
    t = hk*(1/2 * f(a) + sum(functionValues) + 1/2 * f(b));
end

function m = midPointRule(a, b, k, f)
    hk = computeHK(a, b, k);
    r = 1:2^k;
    functionValues = arrayfun(f, a + (r - 1/2) * hk);
    m = hk * sum(functionValues);
end

function hk = computeHK(a, b, k)
    hk = (b-a)/2^k;
end
```

(c) Running code on function $f(x) = e^x/x$ on the interval $(1, 2)$.

```
% create function to be integrated
f = @(x) exp(x)/x;

% set bounds
```

```
a = 1;
b = 2;
n = 10;

% find romberg array for function f
T = NumericalAnalysis.rombergIntegration(a, b, n, f);

% print results
fprintf('     i          T(i,1)            T(i,i) \n');
for i=1:n
    fprintf('%6.0f %19.15f %19.15f \n', i, T(i,1), T(i,i));
end
```

Output generated

```
>> H03
     i          T(i,1)              T(i,i)
     1   3.206404938962185   3.206404938962185
     2   3.068704101194839   3.059524045343683
     3   3.061519689433579   3.061435517910511
     4   3.059717728013521   3.059697224270367
     5   3.059266861956402   3.059265136834889
     6   3.059154121802282   3.059153985140233
     7   3.059125935283745   3.059125924984416
     8   3.059118888561571   3.059118887809404
     9   3.059117126875244   3.059117126821492
    10   3.059116686453301   3.059116686449520
```

Both the trapezoidal rule and the Romberg integration converge very rapidly. I would say that the Romberg integration converged slightly better than the trapezoidal rule by itself.