Math 552 **Introduction to Scientific Computing** **Spring 2020**

SOLUTIONS: Homework Set 1

1. (A result concerning Lagrange polynomials) Consider a set $\{x_0, x_1, \ldots, x_n\}$ of $n+1$ *distinct* points, and the corresponding Lagrange basis functions $\{l_0(x), l_1(x), \ldots, l_n(x)\}$. Prove that

$$\sum_{k=0}^{n} l_k(x) = 1\,.$$

(Hint - Consider interpolating the function $f(x) = 1$, a polynomial of degree 0, at the points $\{x_0, x_1, \ldots, x_n\}$.)

<u>ANS</u>: As the hint suggests, let $f(x) = 1$. The Lagrange form of the polynomial $p_n(x)$ of degree less than or equal to n that interpolates $f(x)$ at the $n+1$ points $\{x_i\}_{i=0}^{n}$ is

$$p_n(x) = \sum_{k=0}^{n} f(x_k) l_k(x) = \sum_{k=0}^{n} 1 * l_k(x) = \sum_{k=0}^{n} l_k(x)\,.$$

Now consider the polynomial $p(x) = p_n(x) - 1$, which has degree $\leq n$. But $p(x_i) = p_n(x_i) - 1 = 0$ since $p_n(x)$ interpolates $f(x) = 1$ at the points $x_i, i = 0, \ldots, n$. This implies that $p(x)$ has **at least** $n+1$ roots. Since $deg(p(x)) \leq n$, by the Fundamental Theorem of Algebra it can have at most n roots unless it is the zero polynomial, so we have $p(x) \equiv 0$ In other words

$$p_n(x) = \sum_{k=0}^{n} l_k(x) = 1\,,$$

for every value of x.

2. Let $f(x) = 1/x$. Take $x_0 = 2$, $x_1 = 3$, $x_2 = 4$.

(a) Find the Lagrange form and standard form of the interpolating polynomial $P_2(x)$ of $f(x)$ at the given interpolation points. Expand out the Lagrange form to verify that it agrees with the standard form of $P_2(x)$ that you found. Also, verify that $P_2(x_i) = f(x_i)$ for $0 \le i \le 2$.

(b) Use the theorem stated in class to find an upper bound for the error

$$||f - P_2||_\infty = \max_{2\le x\le 4} |f(x) - P_2(x)|\,.$$

(c) Find $||f - P_2||_\infty$ to at least 5 decimal places of accuracy.

<u>**ANS**</u>:

(a) The **Lagrange** form is

$$\begin{aligned}
P_2(x) &= \sum_{k=0}^{2} f(x_k) l_k(x) \\
&= f(x_0)\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \\
&= \frac{1}{2}\frac{(x-3)(x-4)}{(2-3)(2-4)} + \frac{1}{3}\frac{(x-2)(x-4)}{(3-2)(3-4)} + \frac{1}{4}\frac{(x-2)(x-3)}{(4-2)(4-3)}\,.
\end{aligned}$$

For the **standard** form we simplify the above expression, giving

$$\begin{aligned}
P_2(x) &= \frac{1}{4}(x-3)(x-4) - \frac{1}{3}(x-2)(x-4) + \frac{1}{8}(x-2)(x-3) \\
&= \frac{1}{4}(x^2-7x+12) - \frac{1}{3}(x^2-6x+8) + \frac{1}{8}(x^2-5x+6) \\
&= \frac{1}{24}x^2 - \frac{3}{8}x + \frac{13}{12}\,.
\end{aligned}$$

Checking

$$\begin{aligned}
P_2(x_0) = P_2(2) &= \frac{1}{24}*2^2 - \frac{3}{8}*2 + \frac{13}{12} = \frac{1}{6} - \frac{3}{4} + \frac{13}{12} = \frac{1}{2} = f(x_0)\,, \\
P_2(x_1) = P_2(3) &= \frac{1}{24}*3^2 - \frac{3}{8}*3 + \frac{13}{12} = \frac{3}{8} - \frac{9}{8} + \frac{13}{12} = \frac{8}{24} = \frac{1}{3} = f(x_1)\,, \\
P_2(x_2) = P_2(4) &= \frac{1}{24}*4^2 - \frac{3}{8}*4 + \frac{13}{12} = \frac{2}{3} - \frac{3}{2} + \frac{13}{12} = \frac{3}{12} = \frac{1}{4} = f(x_2)\,.
\end{aligned}$$

Then $P_2(x) = 1/2 - 1/6(x-2) + 1/24(x-2)(x-3)$ which when expanded gives the same polynomial as above.

(b) Using the error expression for polynomial interpolation, for each $2 \le x \le 4$

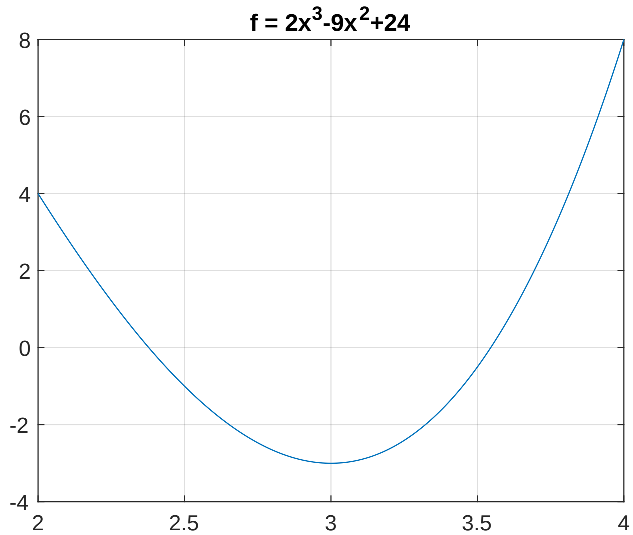
$$|f(x) - P_2(x)| = \frac{|f^3(\xi)|}{3!}\left|\prod_{k=0}^{2}(x-x_k)\right|,$$

for some ξ in $[2,4]$. First we bound $\left|\prod_{k=0}^{2}(x-x_k)\right| = |(x-2)(x-3)(x-4)|$. Let $g(x)=(x-2)(x-3)(x-4)$, then $g'(x)=3x^2-18x+26$, whose roots are $x=3\pm 1/\sqrt{3}$. Plugging each into $g(x)$ and taking the absolute value gives the same value, which is approximately 0.38490017945975, so I'll use $0.4=2/5$ as a bound for $|g(x)|$ over $[2,4]$. Then

$$||f-P_2||_\infty = \max_{2\le x\le 4}|f(x)-P_2(x)| \le \frac{1}{6}\max_{2\le\xi\le 4}|f^3(\xi)|*\frac{2}{5} = \frac{1}{15}\max_{2\le\xi\le 4}\left|\frac{6}{x^4}\right| = \frac{1}{15}\frac{6}{16} = \frac{1}{40},$$

so an upper bound on the error is $1/40 = 0.025$.

(c) This is a standard calculus problem. Let $g(x) = f(x) - P_2(x) = \frac{1}{x} - \left(\frac{1}{24}x^2 - \frac{3}{8}x + \frac{13}{12}\right)$. To find the maximum, we have to check where $g'(x)=0$ in $[2,4]$, and the endpoints $x=2,4$. We have $g'(x) = -\frac{1}{x^2} - \frac{1}{12}x + \frac{3}{8} = -\frac{2x^3-9x^2+24}{24x^2}$. Then $g'(x)=0$ iff $2x^3-9x^2+24=0$. Here is a plot of $2x^3-9x^2+24$ over $[2,4]$: There are clearly



two points in $[2,4]$ at which $2x^3-9x^2+24=0$. How do we find them? Well, they are **roots** of a nonlinear equation. How about Newton's method! Choosing the intial guess x_0 for each root using the graph,

```
>> r1 = mynewton('2*x^3-9*x^2+24','6*x^2-18*x',2.4,1e-14,50);

           x_n                        f(x_n)
 ------------------------------------------------
   2.400000000000000e+00    -1.919999999999966e-01
   2.377777777777778e+00     2.644718792858214e-03
   2.378075705879444e+00     4.675283058475088e-07
   2.378075758565229e+00     1.421085471520200e-14
   2.378075758565231e+00    -3.552713678800501e-15


>> r2 = mynewton('2*x^3-9*x^2+24','6*x^2-18*x',3.6,1e-14,50);
```

```
         x_n                              f(x_n)
------------------------------------------------
 3.600000000000000e+00     6.719999999999970e-01
 3.548148148148148e+00     3.359772392420268e-02
 3.545269033821574e+00     1.018185464545240e-04
 3.545260255416634e+00     9.456471161684021e-10
 3.545260255335102e+00                         0
 3.545260255335102e+00                         0
```

So we take $r1 = 2.378075758565231$ and $r2 = 3.545260255335102$. Now, checking the endpoints, $g(2) = g(4) = 0$. They have to since f and P_2 agree at these points! Also, $g(r1) = -6.682053593859927e{-}03$ and $g(r2) = 4.503073410654312e{-}03$. Thus,

$$||f - P_2||_\infty = \max_{2 \le x \le 4} |f(x) - P_2(x)| \approx 6.682053593859927e{-}03\,.$$

Note, in line with theory, this is less than the upper bound of $1/40 = 0.025$ found in part (b).

3. Approximate the following definite integrals using the composite Trapezoidal rule $T(h)$ for $N = 2, 4, 8, 16, 32$ and 64, where $h = (b-a)/N$.

   (a) $\int_0^2 3x + 1\ dx$

   (b) $\int_0^2 xe^{-x^2}\ dx$

   (c) $\int_0^{2\pi} \cos x + 1\ dx$

   To do so, write an M-file *trap.m*, the first line of which should be

```
function y = my_trap(f,a,b,N)
```

   Include a copy of your code. For each of the functions above make a table, as was done in class, with columns for N, h, $T(h)$, $|\text{error}|$, and $|\text{error}|/h^2$. Are the numbers in the last column converging, and if so, what does it mean? Specifically, comment on the behavior of the error for (a) and (b). If your code is correct, you'll notice that for (c) the last column is not converging, and that the approximation is very accurate. Can you explain why?

   ANS: Here are the results:

(a)

N	h	T(h)	err	err/h^2
2.0000e+00	1.0000e+00	8.0000e+00	0	0
4.0000e+00	5.0000e-01	8.0000e+00	0	0
8.0000e+00	2.5000e-01	8.0000e+00	0	0
1.6000e+01	1.2500e-01	8.0000e+00	0	0
3.2000e+01	6.2500e-02	8.0000e+00	0	0
6.4000e+01	3.1250e-02	8.0000e+00	0	0

(b)

N	h	T(h)	err	err/h^2
2.0000e+00	1.0000e+00	3.8620e-01	1.0465e-01	1.0465e-01
4.0000e+00	5.0000e-01	4.6685e-01	2.3995e-02	9.5980e-02
8.0000e+00	2.5000e-01	4.8494e-01	5.9053e-03	9.4485e-02
1.6000e+01	1.2500e-01	4.8937e-01	1.4708e-03	9.4133e-02
3.2000e+01	6.2500e-02	4.9047e-01	3.6737e-04	9.4046e-02
6.4000e+01	3.1250e-02	4.9075e-01	9.1821e-05	9.4025e-02

(c)

N	h	T(h)	err	err/h^2
2.0000e+00	3.1416e+00	6.2832e+00	0	0
4.0000e+00	1.5708e+00	6.2832e+00	0	0
8.0000e+00	7.8540e-01	6.2832e+00	0	0
1.6000e+01	3.9270e-01	6.2832e+00	1.7764e-15	1.1519e-14
3.2000e+01	1.9635e-01	6.2832e+00	0	0
6.4000e+01	9.8175e-02	6.2832e+00	0	0

   In (a) we expect the Trapezoidal method to perform well since $f''(x) \equiv 0$, so the method is exact! For (b), one sees that err/h^2 is approaching a constant which indicates the expected second order convergence in this example. For (c), even though $f''(x)$ is not identically zero, we see that, except for roundoff when $N = 16$, the method is again exact. The reason is that the Trapezoidal method is particularly accurate when the integrand is a *periodic* function which is the case here.

Here is the code:

```
function y = my_trap(f,a,b,N)
%
h = (b-a)/N;  % grid spacing
x = a:h:b;    % grid points

fval = f(x);
y = (h/2)*(fval(1)+2*sum(fval(2:N))+ fval(N+1));
end
f
```

4. (Corrected Trapezoidal Rule) Recall that one form of the error term for the composite Trapezoidal rule $T(h)$ is

$$E(h) = -\frac{h^3}{12}\sum_{i=0}^{N-1} f''(\eta_i) = -\frac{h^2}{12}\left(\sum_{i=0}^{N-1} f''(\eta_i)h\right), \tag{1}$$

where $\eta_i \in [x_i, x_{i+1}]$, $x_i = a + ih$, and $h = (b-a)/N$. Note that the last term in the parentheses above in (1) can be viewed as a Riemann Sum approximation of

$$\int_a^b f''(x)dx = f'(b) - f'(a).$$

This suggests we could *correct* (more precisely improve) the accuracy of the Trapezoidal Rule by including this term if the values of $f'(a)$ and $f'(b)$ are available. The resulting numerical integration rule is called the Corrected Trapezoidal Rule, whose composite form is given by

$$CT(h) = \frac{h}{2}\left(f(x_0) + 2f(x_1) + \ldots + 2f(x_{N-1}) + f(x_N)\right) - \frac{h^2}{12}(f'(b) - f'(a)).$$

It can be shown that the error for $CT(h)$ when approximating $\int_a^b f(x)dx$ is proportional to h^4, a significant improvement over composite $T(h)$, whose error is proportional to h^2.

(a) Write a MATLAB function M-file to compute $CT(h)$, where the first line is of the form:

```
function y = corrected_trap(f,a,b,N,fpa,fpb)
```

Include a copy of your code.

(b) To numerically verify the order of $CT(h)$ apply your code to approximate

$$I = \int_0^2 xe^{-x^2}dx$$

for $N = 2, 4, 8, 16, 32, 64$. Make a table, as was done in class, with columns for N, h, $CT(h)$, |error|, and |error|$/h^4$. Are the numbers in the last column converging, and if so, what does it mean?

<u>ANS</u>: Here is the table and code:

N	h	CT(h)	err	err/h^4
2.0000e+00	1.0000e+00	4.8021e-01	1.0630e-02	1.0630e-02
4.0000e+00	5.0000e-01	4.9035e-01	4.9066e-04	7.8506e-03
8.0000e+00	2.5000e-01	4.9081e-01	2.9211e-05	7.4779e-03
1.6000e+01	1.2500e-01	4.9084e-01	1.8052e-06	7.3940e-03
3.2000e+01	6.2500e-02	4.9084e-01	1.1251e-07	7.3735e-03
6.4000e+01	3.1250e-02	4.9084e-01	7.0270e-09	7.3684e-03

```
   function y = my_ctrap(f,a,b,fpa,fpb,N)
%
h = (b-a)/N;  % grid spacing
x = a:h:b;    % grid points

fval = f(x);
y = (h/2)*(fval(1)+2*sum(fval(2:N))+ fval(N+1)) ...
    -h^2*(fpb-fpa)/12;
end
```

We see that the error is going to zero, and that the last column is converging to a fixed number. This indicates that the Corrected Trapezoidal method is indeed $O(h^4)$.