Note: open the 'bookmarks' tab of this pdf, you can find links to embedded files ;)

1 Question 1

1.1 (a)
Using the romberg.m script embedded in this pdf, we get that $R_{1,1} \ldots R_{5,1}$ are: 62.437, 57.288, 56.444, 56.263, 56.219.

1.2 (b)
$R_{2,2} \ldots R_{5,5}$ are: 55.5723, 56.2015, 56.2056, 56.2041.

1.3 (c)
$R_{6,1} \ldots R_{6,6}$ are: 58.3627 59.0773, 59.2689, 59.3175, 59.3297, 59.3328.

1.4 (d)
$R_{7,7} \ldots R_{10,10}$ are: 58.4220930, 58.4707174, 58.4704791, 58.4704691.

1.5 (e)
We use the Matlab integration command quadcc with tolerance $10^{-20}$ to get a result, denoted by $R_0$. We regard $R_0$ as the correct result, and plot the log of the absolute error in $R_{i,i}$ in figure 1. From this we can see that the error in $R_{k,k}$ for $k \leq 4$ are not decreasing.

![Figure 1: Error for Romberg integration.](image)

This difficulty for the Romberg integration can be explained from two perspectives. First, our error formula for $R_{k,k}$ is $e_k = O(h_k^{2k})$, provided that the derivatives of the integrand does not grow crazily fast with $k$. In our current problem the length of the integration interval is $b - a = 48$, which is much larger than 1. $h_k = (b - a)/2^{k-1}$, so for $e_{k+1} \leq e_k$, we should have $h_k^{2k+2} \leq h_k^{2k}$. This
implies we should have \( b - a \leq 4^k \) to have our error start decreasing. In our problem this means \( k \geq 3 \).

Another perspective is due to the function we are integrating, \( f(x) = \sqrt{1 + \cos^2(x)} \) is a function with period \( \pi \). Our integration domain has span 48, which equals 15.28 periods. For \( k = 2 \), we are adding a data point at \( x = 24 = 7.64 \pi \), by the periodicity, this equals to adding the point at \( x = 0.64 \pi \). For \( k = 5 \), we have in total \( 2^4 + 1 = 17 \) data points on interval \([0, 48]\): moving these data points to their equivalence in \([0, \pi]\), their locations are shown in figure 2. As we can see, the equivalent locations of the data points in one period \([0, \pi]\) is not evenly distributed: this causes our data not reflecting the function well.

These two perspectives all point us to break the entire interval to smaller periodic segments. In fact, it is even better if we notice that within one period, say on \([0, \pi]\), \( f(x) \) is symmetric about \( \pi/2 \). So we compute the following integration:

\[
\int_{0}^{48} f(x) = 30 \int_{0}^{\pi/2} f(x) + \int_{15\pi}^{48} f(x)
\]

### 2 Question 2

#### 2.1 (a)

First use \( x^{-x} = e^{-x \ln x} \) and expand the exponential function in Taylor series, we get

\[
\int_{0}^{1} x^{-x} \, dx = \int_{0}^{1} e^{-x \ln x} \, dx = \int_{0}^{1} \sum_{k=0}^{\infty} \frac{1}{k!} (-x)^k (\ln x)^k \, dx = \sum_{k=0}^{\infty} \frac{1}{k!} \int_{0}^{1} (-x)^k (\ln x)^k \, dx,
\]

where the change in order of summation and integration is because \( x \ln x \) is bounded on \([0, 1]\), hence the summation converges uniformly on \([0, 1]\). Make the substitution \( u = -\ln x \), then \( x = e^{-u} \),
\[ dx = -x du, \text{ and the integration becomes} \]

\[
\sum_{k=0}^{\infty} \frac{1}{k!} \int_{0}^{1} (-x)^k (\ln x)^k \, dx = \sum_{k=0}^{\infty} \frac{1}{k!} \int_{0}^{1} (-x)^{k+1} (-u)^k \, du \\
= \sum_{k=0}^{\infty} \frac{1}{k!} \int_{0}^{\infty} e^{-u(k+1)} u^k \, du = \sum_{k=0}^{\infty} \frac{1}{k!(k+1)^k} \int_{0}^{\infty} e^{-u(k+1)} [(k+1)u]^k \, du.
\]

Make the substitution \( t = (k+1)u \) the integration becomes

\[
\sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{1}{(k+1)^k} \int_{0}^{\infty} e^{-t^k} \, dt = \sum_{k=0}^{\infty} \frac{1}{(k+1)!(k+1)^k} \Gamma(k + 1).
\]

Through integration by parts, we can see \( \Gamma(k + 1) = k \Gamma(k) \). With the knowledge that \( \Gamma(1) = \int_{0}^{\infty} e^{-t} \, dt = 1 \), we can see \( \Gamma(k + 1) = k! \). Indeed, \( \Gamma \) is the usual Gamma function. The final expression is

\[
\sum_{k=0}^{\infty} \frac{1}{(k+1)^{k+1}} = \sum_{n=1}^{\infty} \frac{1}{n^n}.
\]

2.2 (b)

Write

\[
\int_{0}^{1} x^{-x} \, dx = S_N + R_N,
\]

where for any integer \( N \geq 1 \),

\[
S_N = \sum_{n=1}^{N} n^{-n}, \quad R_N = \sum_{n=N+1}^{\infty} n^{-n}.
\]

We need to choose \( N \geq 1 \) such that \( R_N < 10^{-12} \), which will guarantee that the finite sum \( S_N \) approximates the integral up to twelve digits of accuracy.

Consider the ratio of successive terms.

\[
\frac{(n + 1)^{-(n+1)}}{n^{-n}} = n^{-1} \frac{(n + 1)^{-(n+1)}}{n^{-(n+1)}} = n^{-1} \left(1 + \frac{1}{n}\right)^{-(n+1)}
\]

For \( n \geq 1 \) the second term \( (1 + 1/n)^{-(n+1)} \) is (crudely) bounded by one for example. Therefore

\[
\frac{(n + 1)^{-(n+1)}}{n^{-n}} \leq n^{-1}.
\]

Furthermore \( n^{-1} \) is a decreasing sequence, so if \( n \geq N + 1 \), then the ratio between successive terms is bounded by \( (N + 2)^{-1} \). Therefore

\[
\sum_{n=N+1}^{\infty} n^{-n} \leq (N + 1)^{-(N+1)} \sum_{j=0}^{\infty} (N + 2)^{-j}.
\]

The geometric sum on the right hand side converges for \( N \geq 0 \),

\[
(N + 1)^{-(N+1)} \sum_{j=0}^{\infty} (N + 2)^{-j} = \frac{N + 2}{N + 1} (N + 1)^{-(N+1)}
\]
This shows that
\[ R_N \leq (N + 2)(N + 1)^{-N+2}, \]
and hence \( R_N < 10^{-12} \) if \( N \geq 11 \). Calculating \( S_{11} \) gives the approximation
\[ \int_0^1 x^{-x} \, dx \approx 1.291285997062548 \]

2.3 (c)
If \( I_{j,k}(f) \) is the \((j,k)\) entry in the Romberg table, then the truncation error is of order \( O(h^{2k+2}) \), where \( h = (b - a)/2^j \), provided the even derivatives of \( f \) are bounded in \([a,b]\). In our example, \([a,b] = [0,1]\) and \( f(x) = x^{-x} \), but notice that the derivatives of \( x^{-x} \) are unbounded near zero. This indicates that an order of magnitude approximation using \( \approx h^{2k+2} \) as your error could be misleading. Indeed, to make
\[ (2^{-k})^{2k+2} = 2^{-2k^2 - 2k} \approx 10^{-12} \]
one can take \( k = 4 \). On the other hand, doing the Romberg integration shows that you need to take \( k = 19 \) (the table is too large to fit here).

3 Question 3

(a) Find an exact formula for the cubic polynomial \( P_3(x) = x^3 + \cdots \) such that
\[ \int_{-1}^{1} P_3(x) q(x) \, dx = 0 \]
for any quadratic polynomial \( q \).

(b) Find exact formulas for the three roots \( x_1, x_2, x_3 \) of the equation \( P_3(x) = 0 \).

(c) Find exact formulas for the integration weights \( w_1, w_2, w_3 \) such that
\[ \int_{-1}^{1} q(x) \, dx = \sum_{j=1}^{3} w_j q(x_j) \]
extactly whenever \( q \) is a polynomial of degree 5.

(d) Given any real numbers \( a < b \), find exact formulas for points \( y_j \in [a,b] \) and weights \( u_j > 0 \) such that
\[ \int_{a}^{b} q(x) \, dx = \sum_{j=1}^{3} u_j q(y_j) \]
whenever \( q \) is a polynomial of degree 5.

(e) Explain why each of the three factors in the error estimate
\[ \int_{a}^{b} f(x) \, dx - \sum_{j=1}^{3} u_j f(y_j) = C_0 f^{(6)}(\xi) \int_{a}^{b} (y - y_1)^2 (y - y_2)^2 (y - y_3)^2 \, dy \]
is inevitable and determine the exact value of the constant \( C_0 \).
(f) Use your code from Question 2 to evaluate
\[ E_6 = \int_0^1 (x - x_1)^2(x - x_2)^2(x - x_3)^2 \, dx \]
to 3-digit accuracy.

3.1 (a)
In class we constructed polynomials \( P_0(x) = 1, \) \( P_1(x) = x, \) and
\[ P_2(x) = xP_1(x) - \frac{1}{3}P_0(x) = x^2 - \frac{1}{3} \]
such that \( \int P_jq \, dx = 0 \) whenever \( q \) had lower degree than \( P_j. \) Since each \( P_j \) begins with \( x^j, \) the \( P_j's \) form a basis for quadratic polynomials. Hence we seek \( P_3(x) = xP_2(x) - cP_1(x) \) where \( c \) is chosen to make
\[ 0 = \int_{-1}^{1} P_3(x) \cdot P_0(x) \, dx = \int_{-1}^{1} P_3(x) \cdot P_1(x) \, dx = \int_{-1}^{1} P_3(x) \cdot P_2(x) \, dx. \]
Here \( P_0 \) and \( P_2 \) are automatic by parity since \( P_3 \) is odd and they are even. So \( c \) must satisfy
\[ \int_{-1}^{1} (xP_2(x) - cP_1(x))P_1(x) \, dx = 0 \]
or
\[ c = \frac{\int_{-1}^{1} xP_2(x)P_1(x) \, dx}{\int_{-1}^{1} P_1(x)^2 \, dx} = \frac{\int_{-1}^{1} x^4 - \frac{1}{3}x^2 \, dx}{\int_{-1}^{1} x^2 \, dx} = \frac{8}{\frac{2}{3}} = \frac{4}{15}. \]
Thus
\[ P_3(x) = x^3 - \frac{3}{5}x = \frac{5x^3 - 3x}{5}. \]

3.2 (b)
We can factor \( P_3(x) = x \left(x^2 - \frac{3}{5}\right) \) so that the roots (in order) are
\[ x_1 = -\sqrt{\frac{3}{5}}, x_2 = 0, x_3 = \sqrt{\frac{3}{5}}. \]

3.3 (c)
Since the rule is accurate for degree-5 polynomials we must have a fortiori
\[ \int_{-1}^{1} L_j(x) \, dx = \sum_{k=1}^{3} w_k L_j(x_k) = w_j \]
for each quadratic Lagrange basis polynomial
\[ L_j(x) = \frac{\prod_{k \neq j} (x - x_k)}{\prod_{k \neq j} (x_j - x_k)}. \]
It is also true that
\[ \int_{-1}^{1} L_j^2(x) \, dx = \sum_{k=1}^{3} w_k L_j^2(x_k) = w_j \]
which is convenient for numerical integration because all values are positive, but less convenient for hand computation since the degree doubles. Hence we integrate by parts to obtain
\[ \int_{-1}^{1} x L_j(x) \, dx = \left. x L_j(x) - \frac{x^2}{2} L_j'(x) + \frac{x^3}{3!} L_j''(x) \right|_{-1}^{1} \]
Since
\[ L_1(x) = \frac{5}{6} x \left( x - \sqrt{\frac{3}{5}} \right), \quad L_2(x) = -\frac{5}{3} \left( x^2 - \frac{3}{5} \right), \quad L_3(x) = \frac{5}{6} x \left( x + \sqrt{\frac{3}{5}} \right) \]
we can compute
\[ \int_{-1}^{1} L_1(x) \, dx = \frac{5}{36} x^2 \left( 2x - 3 \sqrt{\frac{3}{5}} \right) \bigg|_{-1}^{1} = \frac{10}{36} - \left( -\frac{10}{36} \right) = \frac{5}{9} = w_1 \]
\[ \int_{-1}^{1} L_2(x) \, dx = \left( x - \frac{5}{9} x^3 \right) \bigg|_{-1}^{1} = \frac{4}{9} - \left( -\frac{4}{9} \right) = \frac{8}{9} = w_2 \]
\[ \int_{-1}^{1} L_3(x) \, dx = \frac{5}{36} x^2 \left( 2x + 3 \sqrt{\frac{3}{5}} \right) \bigg|_{-1}^{1} = \frac{10}{36} - \left( -\frac{10}{36} \right) = \frac{5}{9} = w_3 \]

3.4 (d)

The change of variables
\[ x \mapsto y = \frac{a + b}{2} + \frac{b - a}{2} \]
sends the interval \([-1, 1]\) to \([a, b]\). The change of variable \(dy = \frac{b - a}{2} \, dx\) tells us that
\[ \int_{a}^{b} f(y) \, dy = \frac{b - a}{2} \int_{-1}^{1} g(x) \, dx \]
where \(g(x) = f \left( \frac{a+b}{2} + x \frac{b-a}{2} \right)\) is a polynomial of the same degree as \(f\).

Since the transformation \(x \mapsto y\) preserves polynomial degree we can re-use our weights from the previous parts.
\[ \int_{a}^{b} f(y) \, dy = \frac{b - a}{2} \int_{-1}^{1} g(x) \, dx = \frac{b - a}{2} \left[ w_1 g(x_1) + w_2 g(x_2) + w_3 g(x_3) \right] \]
This means we can use the weights
\[ u_j = \frac{b - a}{2} w_j \]
(we have \(u_j > 0\) since \(b > a, w_j > 0\)) and the values \(g(x_j) = f \left( \frac{a+b}{2} + x_j \frac{b-a}{2} \right)\) mean we can use the nodes
\[ y_j = \frac{a + b}{2} + x_j \frac{b-a}{2} \]
3.5 (e)

Gaussian quadrature with three nodes can be seen as arising from a Hermite interpolation, but a very special one. If we interpolate

\[ H(x) = H_1(x)f(x_1) + H_2(x)f(x_2) + H_3(x)f(x_3) + \hat{H}_1(x)f'(x_1) + \hat{H}_2(x)f'(x_2) + \hat{H}_3(x)f'(x_3) \]

and then approximate

\[ \int_{-1}^{1} f(x) \, dx \approx \int_{-1}^{1} H(x) \, dx \]

\[ = f(x)I_1 + f(x_2)I_2 + f(x_3)I_3 + f'(x_1)\hat{I}_1 + f'(x_2)\hat{I}_2 + f'(x_3)\hat{I}_3 \]

where

\[ I_j = \int_{-1}^{1} H_j(x) \, dx, \quad \hat{I}_j = \int_{-1}^{1} \hat{H}_j(x) \, dx. \]

Gaussian quadrature corresponds to the unique choice\(^1\) \( x_1 < x_2 < x_3 \) such that

\[ \hat{I}_1 = \hat{I}_2 = \hat{I}_3 = 0. \]

This allows \( \int_{-1}^{1} f(x) \, dx \) to be approximated without the ability to compute \( f'(x_0) \) for any particular value.

One can check that \( I_1 = I_3 = \frac{5}{9}, \, I_2 = \frac{8}{9} \) and \( \hat{I}_1 = \hat{I}_2 = \hat{I}_3 = 0. \)

From our approximation, we have

\[ f(x) - H(x) = \frac{f^{(6)}(\xi(x))}{6!}(x-x_1)^2(x-x_2)^2(x-x_3)^2 \]

for \( \xi(x) \in (-1,1) \). The \( I_j \) and \( \hat{I}_j \) values mentioned above mean that

\[ \int_{-1}^{1} H(x) \, dx = \frac{5}{9}f(x_1) + \frac{8}{9}f(x_2) + \frac{5}{9}f(x_3) \]

hence integrating the error term above

\[ \int_{-1}^{1} f(x) \, dx - \left[ \frac{5}{9}f(x_1) + \frac{8}{9}f(x_2) + \frac{5}{9}f(x_3) \right] = \int_{-1}^{1} \frac{f^{(6)}(\xi(x))}{6!}(x-x_1)^2(x-x_2)^2(x-x_3)^2 \, dx. \]

\(^1\) One can verify that it is unique by solving a system of three polynomials in \( x_1, x_2, x_3 \). For example, \( \hat{I}_1 = 0 \) gives a polynomial by computing

\[ \int_{-1}^{1} (x-x_1)(x-x_2)^2(x-x_3)^2 \, dx = 0. \]

Values that satisfy \( \hat{I}_1 = \hat{I}_2 = \hat{I}_3 = 0 \) form an ideal \( I \) in \( \mathbb{Q}[x_1, x_2, x_3] \). Solutions where \( x_1, x_2, x_3 \) are not unique will live in one of the ideals \( J_{ij} = (x_i - x_j) \) (corresponding to \( x_i = x_j \)). Thus we consider the saturation ideal

\[ M = (((I : J_{12}^{\infty}) : J_{23}^{\infty}) : J_{31}^{\infty}) \]

to find unique solutions. Using the Gröbner basis for \( M \) we find solutions must satisfy

\[ 5x_3^3 - 3x_3 = 5x_2^2 + 5x_2x_3 + 5x_2^2 - 3 = x_1 + x_2 + x_3 = 0 \]

which gives exactly the six permutations of \( \left( -\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}} \right) \).
Since \((x - x_1)^2(x - x_2)^2(x - x_3)^2\) is non-negative theorem, the mean value theorem for integrals can be applied and we find

\[
\int_{-1}^{1} \frac{f^{(6)}(\xi(x))}{6!} (x - x_1)^2(x - x_2)^2(x - x_3)^2 \, dx = \frac{f^{(6)}(\xi)}{6!} \int_{-1}^{1} (x - x_1)^2(x - x_2)^2(x - x_3)^2 \, dx
\]

for a fixed value \(\xi \in (-1, 1)\).

Why are each of the factors in the error estimate inevitable?

- The integral is inevitable because Gaussian quadrature is equivalent to integrating a Hermite interpolating polynomial. Also, the integrand is a polynomial of degree 6 for which the Gaussian integration gives 0 and the integral is positive. Hence testing Gaussian integration on this integrand shows that the error must be proportional to this integral.
- The sixth derivative is inevitable because the error is zero whenever the integrand \(f\) is a polynomial of degree 5 or less.
- The coefficient \(C_6\) is inevitable because the sixth derivative of the integrand in the integral factor introduces a factor of \(6!\).

We’ve only shown that \(C_6 = \frac{1}{6!}\) in the case that \(a = -1, b = 1\) but this is actually true for any choice of \(a, b\).

To see this, we’ll use our transformation \(y = \frac{a + b}{2} + x \frac{b - a}{2}\) and \(g(x) = f(y)\). Then

\[
g^{(6)}(x) = f^{(6)}(y) \frac{dy}{dx}^6 = f^{(6)}(y) \left(\frac{b - a}{2}\right)^6
\]

and

\[
y - y_j = \frac{b - a}{2}(x - x_j) \implies (y - y_1)^2(y - y_2)^2(y - y_3)^2 = \left(\frac{b - a}{2}\right)^6 (x - x_1)^2(x - x_2)^2(x - x_3)^2.
\]

Thus, our error is given by

\[
\int_{a}^{b} f(y) \, dy - [u_1f(y_1) + u_2f(y_2) + u_3f(y_3)]
\]

\[
= \left(\frac{b - a}{2}\right) \left(\int_{-1}^{1} g(x) \, dx - [w_1g(x_1) + w_2g(x_2) + w_3g(x_3)]\right)
\]

\[
= \left(\frac{b - a}{2}\right) \frac{g^{(6)}(\xi_1)}{6!} \int_{-1}^{1} (x - x_1)^2(x - x_2)^2(x - x_3)^2 \, dx
\]

\[
= \frac{f^{(6)}(\xi_2)}{6!} \int_{-1}^{1} \left(\frac{b - a}{2}\right)^6 (x - x_1)^2(x - x_2)^2(x - x_3)^2 \left(\frac{b - a}{2}\right) \, dx
\]

\[
= \frac{f^{(6)}(\xi_2)}{6!} \int_{-1}^{1} (y - y_1)^2(y - y_2)^2(y - y_3)^2 \, dy
\]

where \(\xi_1 \in (-1, 1)\) implies \(\xi_2 = \frac{a + b}{2} + \xi_1 \frac{b - a}{2} \in (a, b)\).
3.6 (f)

First note that since
\[(x - x_1)(x - x_3) = x^2 - \frac{3}{5}\]
and \((x - x_2)^2 = x^2\) we can compute the integral by hand
\[
E_6 = \int_0^1 x^2 \left(x^2 - \frac{3}{5}\right)^2 \, dx = \int_0^1 x^2 \left(x^4 - \frac{6}{5}x^2 + \frac{9}{25}\right) \, dx
\]
\[
= \frac{x^7}{7} - \frac{6x^5}{5\cdot5} + \frac{9x^3}{25\cdot3}\bigg|_0^1 = \frac{1}{7} - \frac{6}{5\cdot5} + \frac{9}{25\cdot3}
\]
\[
= \frac{25}{175} - \frac{42}{175} + \frac{21}{175} = \frac{4}{175} \approx 0.022857.
\]

Using the “official” gadap.m we find
\[
\text{>> } f = @(x, p) (x^2 * (x^2 - 0.6)^2);
\text{>> } [\text{intVal}, \text{abt}] = \text{gadap}(0, 1, f, \text{NaN}, 1e-3);
\text{>> } \text{format long}
\text{>> intVal}
\]
\[
\text{intVal =}
0.0228515625000000
\]
accurate to 3 digits.

4 Question 4

(a) Write, test and debug an adaptive 3-point Gaussian integration code gadap.m.

(b) Approximate the integral \[\int_0^1 x^{-x} \, dx\] using your code from (a). Measure the total number of function evaluations required to obtain 12-digit accuracy. Plot the accepted intervals.

Compare your results with those obtained in the previous problem set by Romberg integration.

4.1 (a)

See the file embedded in this pdf file.

4.2 (b)

Using the “official” gadap.m script, we can track the number of function evaluations by using WrappedCall.m to keep a count every time the method is called.

classdef WrappedCall < handle
   properties
      count = 0;
      wrappedMethod;
   end
   methods

function obj = WrappedCall(wrappedMethod)
    obj.wrappedMethod = wrappedMethod;
end
function r = f(obj, x, p)
    obj.count = obj.count + 1;
    r = obj.wrappedMethod(x, p);
end
end
end

Using this, we can define a function handle which computes $x^{-x}$ (and doesn’t use the extra parameter \( p \)), then wrap that function handle with a counter and call \texttt{gadap}:

\begin{verbatim}
>> f = @(x, p) (x^(-x));
>> wrapped = WrappedCall(f);
>> [intVal, abt] = gadap(0, 1, @wrapped.f, NaN, 1e-12);
>> wrapped.count
ans =
    1449
>> format long
>> intVal
intVal =
    1.291285997062850
\end{verbatim}

In total there are 1449 function calls vs. about a million for Romberg, and the solution is accurate to 12 digits:

\begin{verbatim}
123456789012
-------------------
1.291285997062850
1.2912859970621850
1.2912859970621663540407...
\end{verbatim}

See Figure 3 for the accepted intervals. Another way to count the function calls is to count the number of intervals and multiply by 3.
Figure 3: Integration Intervals for $x^{-x}$