Assignment 1  
Computing π on Gilligan’s Island

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Do What?

One of the most useful constants is the transcendental number \( \pi \approx 3.141592654 \). It is the ratio of the circumference of a circle to its diameter. Archimedes was the first to calculate its value in the third century B.C. It is both irrational\(^1\) and transcendental. Euler’s formula, \( 1 + e^{i\pi} = 0 \), elegantly expresses the relationship among the five most important constants.

Your task is to find approximations for \( \pi \) using two rather unconventional methods. The first method uses a simple Monte Carlo simulation to derive a value for \( \pi \), while the second uses numerical integration.

Method 1

Suppose that the Professor on Gilligan’s Island needs an approximation of \( \pi \) to three decimal places for his latest invention (which he hopes will impress Mary-Ann enough that she will fix him one of her fabulous banana and coconut pies), but all that he has are a basket of kukui nuts and a length of rope. Since Gilligan is always thwarting his rescue plans, he has a lot of time on his hands and so comes up with the following method.

Imagine that you have a unit square with bottom left corner at the origin \((0, 0)\). On top of that square inscribe a circle with radius 1 and its center at the origin (see Figure 1(a)). Choose two random numbers \( 0 \leq x, y \leq 1 \) and use them as the coordinate of a point in the square. The probability that this point falls inside the circle is \( \pi/4 \).

The Professor remembers enough geometric constructions from high school to use his length of rope to make a primitive compass. He uses this to draw a unit square in the sand beneath a tall palm tree. He then uses it to inscribe a circle of unit radius with its center on the bottom left corner of the square. He now has Gilligan climb the palm tree with the basket of nuts. He has him shake the basket and scatter the nuts over the square. He has the Skipper count the nuts that fall inside the square, and also specifically those that fall in the inscribed quarter circle. The ratio of the number of nuts in the quarter circle to the total number of nuts in the square is his first approximation of \( \pi/4 \).

Since he has a lot of time on his hands, and he really wants that banana and coconut pie, he has Gilligan and the Skipper repeat this experiment many times. He averages the results together to come up with his approximation of \( \pi \).

Since you really don’t have a basket of kukui nuts, or Gilligan and the Skipper to do your work for you, but you do have a computer, an algorithm to simulate it is in order. A simple algorithm to estimate the value of \( \pi \) can be implemented by repeatedly choosing random points and checking whether they fall into the intersection of the quarter circle and the square. The fraction of points that fall into this intersection is \( \pi/4 \). A point \((x, y)\) is in the intersection if \( \sqrt{x^2 + y^2} \leq 1 \).

Let \( X \) be the set of all points that fall in the intersection of the square and circle, that is, \( X = \bigcup_{i=1}^{n} \{ (x_i, y_i) \} \) such that \( \sqrt{x_i^2 + y_i^2} \leq 1 \). As we can see from Figure 1(b), the value \( 4|X|/n \) approaches \( \pi \) as \( n \) gets large. Note that some of these approximations of \( \pi \) will be too large, others will be too small, but none will be exact since you do not have an infinite number of kukui nuts. The law of large numbers tells us that if we average the results of the kukui nut dropping

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\(^1\)It survived a legislative attempt to set \( \pi = 3 \) (see Indiana Engrossed House Bill no. 246, January 1897).
experiments then we will get a better approximation of $\pi$ since $\lim_{n \to \infty} \Pr\{\lfloor X_1 + \cdots + X_n \rfloor / n - \pi/4 \leq \epsilon \} = 1$ for as small an $\epsilon$ as you might care to choose.

In your most elegant FORTRAN, write a program to approximate $\pi$ to three decimal places using this method.

**Method 2**  
Extra Credit

The second method is a bit more conventional. As is usual on Gilligan’s Island, useful items float into the lagoon. During this episode a crate of cheap solar powered calculators wash up on the beach. Notice that the area of the intersection of the square and the circle is $\pi/4$. So, in order to get an approximate value of $\pi$ you could compute

$$\int_0^1 \sqrt{1-x^2} \, dx = \pi/4.$$

As we know from many years of watching Gilligan’s Island, the Professor always seems to have the right book at the right time, in this case it’s his undergraduate numerical analysis text. A numerical approximation of this integral can be obtained using the **trapezoidal rule**

$$\int_a^b f(x) \, dx \approx \frac{b-a}{n} \sum_{i=1}^n f(x_i) + \frac{f(x_{i-1})}{2}.$$

The accuracy of your approximation will depend on your choice of $n$. An even better approximation can be obtained using [Romberg integration](see the description available on the class web page, which is § 4.6 from Burden, Faires & Reynolds, *Numerical Analysis*). In the general case, adaptive algorithms are used to obtain approximations for functions that are not as well-behaved as the one that now interests us.

Again, in your most elegant FORTRAN, write a program that employs both the trapezoidal rule and the Romberg integration to approximate the integral $\int_0^1 \sqrt{1-x^2} \, dx$ to five decimal places and use it to derive an estimate of $\pi$. Be sure to mention the value of $n$ that you had to choose for each rule to achieve the desired precision. In the case of Romberg integration, you should produce a table like Table 4.8 in § 4.6 of Burden et al.

**Due When?**

This assignment will be due at noon on **Thursday, April 4, 2002**. **Monday, October 6, 2003.**
3. Use the Adaptive Quadrature Algorithm to approximate \( \int_{10}^{10} \ln x \, dx \) to within \( 10^{-4} \). Compare your approximation to the result in Exercise 8 of Section 4.4. Compare the number of nodes required in each case.

4. Use the Adaptive Quadrature Algorithm to approximate \( \int_{0}^{1} \{1 + (\cos x)^2\}^{1/2} \, dx \) to within \( 10^{-4} \). Does this technique have any advantage in this instance? (Compare the result and the number of functional evaluations with those of Exercise 13 in Section 4.4).

5. Use the Adaptive Quadrature Algorithm to approximate \( \int_{0}^{1} x^{1/3} \, dx \) to within \( 10^{-4} \). Compare your approximation to the result in Exercise 7(f) of Section 4.3. Compare the number of nodes required in each case.

6. Use the Adaptive Quadrature Algorithm to approximate \( \int_{1}^{1} \sin(1/x) \, dx \) to within \( 10^{-3} \). Sketch the graph of \( f(x) = \sin(1/x) \) on \([1, 1]\).

7. The differential equation

\[
u''(t) + ku(t) = F_0 \cos \omega t
\]
describes a spring-mass system with mass \( m \), spring constant \( k \), and no applied damping. The term \( F_0 \cos \omega t \) describes a periodic external force applied to the system. The solution to the equation when the system is initially at rest (\( u'(0) = u(0) = 0 \)) is

\[
u(t) = \frac{2F_0}{m(\omega_0^2 - \omega^2)} \sin \left( \frac{\omega_0 - \omega}{2} \right) \sin \left( \frac{\omega_0 + \omega}{2} \right) t,
\]
where \( \omega_0 = \frac{F_0}{m} \neq \omega \).

Sketch the graph of \( u \) when \( m = 1, k = 9, F_0 = 1, \omega = 2 \), and \( t \in [0, 2\pi] \). Use both the Adaptive Quadrature method and Simpson's composite rule to determine \( \int_{0}^{2\pi} u(t) \, dt \) to within \( 10^{-4} \).

8. If the term \( cu'(t) \) is added to the left side of the motion equation in Exercise 7, the resulting differential equation describes a spring-mass system that is damped with damping constant \( c \). The solution to this equation, when the solution is initially at rest is

\[
u(t) = c_1 e^{\delta t} + c_2 e^{\delta t} + \frac{F_0}{\sqrt{m^2(\omega_0^2 - \omega^2) + c^2 \omega^2}} \cos (\omega t - \delta)
\]
where

\[
\delta = \arctan \left( \frac{c \omega}{m(\omega_0^2 - \omega^2)} \right), \quad r_1 = \frac{-c + \sqrt{c^2 - 4\omega_0^2 m^2}}{2m},
\]
and

\[
r_2 = \frac{-c - \sqrt{c^2 - 4\omega_0^2 m^2}}{2m}.
\]

Sketch the graph of \( u \) when \( m = 1, k = 9, F_0 = 1, c = 1, \omega = 2 \), and \( t \in [0, 2\pi] \). Use both the Adaptive Quadrature method and Simpson's composite rule to determine \( \int_{0}^{2\pi} u(t) \, dt \) to within \( 10^{-4} \).

### 4.6 Romberg Integration

Although the trapezoidal rule is the easiest Newton–Cotes formula to apply, we have shown repeatedly in the previous sections that it lacks the degree of accuracy generally required. Romberg integration is a method that has wide application because it uses the trapezoidal rule to give preliminary approximations, and then applies the Richardson extrapolation process (discussed in Section 4.2) to obtain improvements of the approximations.
To begin the presentation of the Romberg integration scheme, recall (Theorem 4.5) that the extended trapezoidal rule for approximating the integral of a function $f$ on an interval $[a, b]$ using $m$ subintervals is

$$
\int_{a}^{b} f(x) \, dx = \frac{h}{2} \left[ f(a) + f(b) + 2 \sum_{j=1}^{m-1} f(x_j) \right] - \frac{(b - a)}{12} h^2 f''(\mu)
$$

where $a < \mu < b$, $h = (b - a)/m$ and $x_j = a + jh$ for each $j = 0, 1, \ldots, m$.

The first step in the Romberg process involves obtaining the trapezoidal rule approximations with $m_1 = 1$, $m_2 = 2$, $m_3 = 4$, \ldots, $m_n = 2^{n-1}$ where $n$ is some positive integer. The values of the step size $h_k$ corresponding to $m_k$ will be $h_k = (b - a)/m_k = (b - a)/2^{k-1}$, and with this notation the trapezoidal rule becomes

$$
\int_{a}^{b} f(x) \, dx = \frac{h_k}{2} \left[ f(a) + f(b) + 2 \left( \sum_{i=1}^{2^{k-1} - 1} f(a + ih_k) \right) \right] - \frac{(b - a)}{12} h_k^2 f''(\mu_k)
$$

where $\mu_k$ is a point in $[a, b]$.

If the notation $R_{k,1}$ is introduced to denote that portion of (4.57), which is used for the trapezoidal approximation, then

$$
R_{1,1} = \frac{h_1}{2} \left[ f(a) + f(b) \right] = \frac{(b - a)}{2} \left[ f(a) + f(b) \right];
$$

$$
R_{2,1} = \frac{h_2}{2} \left[ f(a) + f(b) + 2f(a + h_2) \right] = \frac{(b - a)}{4} \left[ f(a) + f(b) + 2f \left( a + \frac{(b - a)}{2} \right) \right] = \frac{1}{2} \left[ R_{1,1} + h_1 f(a + \frac{1}{2}h_1) \right];
$$

$$
R_{3,1} = \frac{h_3}{2} \left\{ f(a) + f(b) + 2 \left[ f \left( a + \frac{(b - a)}{4} \right) + f \left( a + \frac{3(b - a)}{4} \right) \right] \right\} = \frac{(b - a)}{8} \left[ f(a) + f(b) + 2 \left[ f \left( a + \frac{(b - a)}{4} \right) + f \left( a + \frac{3(b - a)}{4} \right) \right] \right] = \frac{1}{2} \left[ R_{2,1} + h_2 \left[ f \left( a + \frac{h_2}{2} \right) + f \left( a + \frac{3h_2}{2} \right) \right] \right];
$$

and, in general,

$$
R_{k,1} = \frac{1}{2} \left[ R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f \left( a + \left( i - \frac{1}{2} \right)h_{k-1} \right) \right]
$$

for each $k = 2, 3, \ldots, n$.

For the derivation of Eq. (4.58), the reader is referred to Exercises 7 and 8.
EXAMPLE 1 Using Eq. (4.58) to perform the first step of the Romberg integration scheme for approximating \( \int_0^\pi \sin x \, dx \) with \( n = 6 \) leads to:

\[
R_{1,1} = \frac{\pi}{2} [\sin 0 + \sin \pi] = 0;
\]

\[
R_{2,1} = \frac{1}{2} \left[ R_{1,1} + \pi \sin \frac{\pi}{2} \right] = 1.57079633;
\]

\[
R_{3,1} = \frac{1}{2} \left[ R_{2,1} + \frac{\pi}{2} \left( \sin \frac{\pi}{4} + \sin \frac{3\pi}{4} \right) \right] = 1.89611890;
\]

\[
R_{4,1} = \frac{1}{2} \left[ R_{3,1} + \frac{\pi}{4} \left( \sin \frac{\pi}{8} + \sin \frac{3\pi}{8} + \sin \frac{5\pi}{8} + \sin \frac{7\pi}{8} \right) \right] = 1.97423160;
\]

\[
R_{5,1} = 1.99357034,
\]

and \( R_{6,1} = 1.99839336. \)

Since the correct value for this integral is 2, it is clear that, although the calculations involved are not difficult, the convergence is very slow.

To speed the convergence the Richardson extrapolation procedure will now be performed. It can be shown, although not easily (seeRalston and Rabinowitz [67], pages 123–126 and accompanying exercises for a presentation), that the extended trapezoidal rule given in Eq. (4.57) can be written with an alternate error term in the form:

\[
\int_a^b f(x) \, dx = \frac{h_k}{2} \left[ f(a) + f(b) + 2 \left( \frac{1}{2} \sum_{i=1}^{2^{k-1}-1} f(a + i h_k) \right) \right] - \frac{h_k^2}{12} [f'(b) - f'(a)] + \frac{(b-a)h_k^4}{720} f^{(4)}(\mu_k),
\]

for each \( k = 1, 2, \ldots, n \) and some \( a < \mu_k < b \).

With the extended trapezoidal rule in this form, we can eliminate the term involving \( h_k^2 \) by combining the equations

\[
\int_a^b f(x) \, dx = R_{k-1,1} - \frac{h_k^2}{12} [f'(b) - f'(a)] + \frac{(b-a)h_k^4}{720} f^{(4)}(\mu_{k-1})
\]

and

\[
\int_a^b f(x) \, dx = R_{k,1} - \frac{h_k^2}{12} [f'(b) - f'(a)] + \frac{(b-a)h_k^4}{720} f^{(4)}(\mu_k)
\]

\[
= R_{k,1} - \frac{h_k^2}{48} [f'(b) - f'(a)] + \frac{(b-a)h_k^4}{720} f^{(4)}(\mu_k)
\]
to obtain

\[
\int_a^b f(x) \, dx = \frac{4R_{k,1} - R_{k-1,1}}{3} + \frac{(b-a)}{2160} \left[ 4h^4 f^{(4)}(\mu_k) - h_{k-1}^4 f^{(4)}(\mu_{k-1}) \right]
\]

\[
= \frac{4R_{k,1} - R_{k-1,1}}{3} + O(h^4).
\]

It is an easy matter to show (see Exercise 6) that the approximation obtained by this technique is actually the approximation given by the Simpson's composite rule with \( h = h_k \), so the error of order \( h^4 \) is expected.

To continue the Romberg scheme, define

\[
R_{k,2} = \frac{4R_{k,1} - R_{k-1,1}}{3}
\]

for each \( k = 2, 3, \ldots, n \), and apply the Richardson extrapolation procedure to these values. It can be shown (see Ralston and Rabinowitz [67]) that the process gives

\[
R_{i,r} = \frac{4^{i-r} R_{i-r,1} - R_{i-r,1}}{4^{i-r} - 1}
\]

for each \( i = 2, 3, 4, \ldots, n \), and \( j = 2, \ldots, i \), where the values with larger \( j \) index correspond to successively higher-order Newton–Cotes formulas. The approximations are often presented in a table of the form of Table 4.7.

<table>
<thead>
<tr>
<th>( R_{1,1} )</th>
<th>( R_{2,1} )</th>
<th>( R_{2,2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R_{3,1} )</td>
<td>( R_{3,2} )</td>
<td>( R_{3,3} )</td>
</tr>
<tr>
<td>( R_{4,1} )</td>
<td>( R_{4,2} )</td>
<td>( R_{4,3} )</td>
</tr>
<tr>
<td>( \vdots )</td>
<td>( \vdots )</td>
<td>( \vdots )</td>
</tr>
<tr>
<td>( R_{n,1} )</td>
<td>( R_{n,2} )</td>
<td>( R_{n,3} )</td>
</tr>
</tbody>
</table>

An elegant summability theorem of Silverman and Toeplitz can be used to show that the terms along the diagonal will converge to the integral provided the values of \( R_{n,1} \) converge to this number. A proof of this result, together with necessary conditions for this convergence, can be found in Ralston and Rabinowitz [67], pages 123–126. It is generally expected that the diagonal sequence \( \{R_{m,m}\}_{m=1}^{\infty} \) converges much more rapidly than \( \{R_{n,1}\}_{n=1}^{\infty} \).

The Romberg technique has the additional desirable feature that it allows an entire new row in the table to be calculated by simply doing one application of the trapezoidal rule and then using the previously calculated values to obtain the succeeding entries in the row. The method generally used to construct a table of this type incorporates this feature by calculating the entries row by row, that is, in the order \( R_{1,1}, R_{2,1}, R_{2,2}, R_{3,1}, R_{3,2}, R_{3,3}, \ldots, R_{n,1}, R_{n,2}, R_{n,3}, \ldots, R_{n,n} \). The following algorithm describes this technique in detail.
Romberg Algorithm 4.3

To approximate the integral \( I = \int_a^b f(x) \, dx \), select an integer \( n > 0 \).

**INPUT** endpoints \( a, b \); integer \( n \).

**OUTPUT** an array \( R \). (\( R_{n,n} \) is the approximation to \( I \). Computed by rows; only 2 rows saved in storage.)

**Step 1** Set \( h = b - a \);
\[ R_{1,1} = h(f(a) + f(b))/2. \]

**Step 2** OUTPUT \( (R_{1,1}) \).

**Step 3** For \( i = 2, \ldots, n \) do Steps 4–8.

**Step 4** Set \( R_{2,1} = \frac{1}{2} \left[ R_{1,1} + h \sum_{k=1}^{2^{i-2}} f(a + (k - .5)h) \right] \)  (Approximation from trapezoidal method.)

**Step 5** For \( j = 2, \ldots, i \)
\[ \text{set } R_{2,j} = \frac{4^{j-1}R_{2,j-1} - R_{1,j-1}}{4^{j-1} - 1}. \]  (Extrapolation.)

**Step 6** OUTPUT \( (R_{2,i} \text{ for } j = 1, 2, \ldots, i) \).

**Step 7** Set \( h = h/2 \).

**Step 8** For \( j = 1, 2, \ldots, i \) set \( R_{1,j} = R_{2,j} \). (Update row 1 of \( R \).)

**Step 9** STOP.

It is often useful not to have predetermined a specific value for \( n \) and instead to modify the algorithm slightly to allow the procedure to continue until a value of \( n \) is found that satisfies \( |R_{n,n} - R_{n-1,n-1}| < \epsilon \) for a given tolerance \( \epsilon \).

**EXAMPLE 2** In Example 1, the values for \( R_{1,1} \) through \( R_{n,1} \) were obtained for approximating \( \int_0^n \sin x \, dx \) with \( n = 6 \). With Algorithm 4.3, the Romberg table is shown in Table 4.8.

**TABLE 4.8**

<table>
<thead>
<tr>
<th>( n )</th>
<th>( R_{1,1} )</th>
<th>( R_{1,2} )</th>
<th>( R_{1,3} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.57079633</td>
<td>2.09439511</td>
<td>1.99857073</td>
</tr>
<tr>
<td>1</td>
<td>1.89611890</td>
<td>2.00455976</td>
<td>1.9998313</td>
</tr>
<tr>
<td>2</td>
<td>1.97423160</td>
<td>2.00026917</td>
<td>1.99999975</td>
</tr>
<tr>
<td>3</td>
<td>1.99357034</td>
<td>2.00001659</td>
<td>1.99999999</td>
</tr>
<tr>
<td>4</td>
<td>1.99839336</td>
<td>2.00000103</td>
<td>2.00000000</td>
</tr>
</tbody>
</table>

**Exercise Set 4.6**

1. Use Romberg integration to calculate \( R_{3,3} \) for the following definite integrals. Compare your results to those obtained in Exercises 1 and 2 of Section 4.4.
   a) \( \int_1^3 \frac{dx}{x} \)
   b) \( \int_0^2 x^3 \, dx \)
c) $\int_0^3 x \sqrt{1 + x^2} \, dx$

d) $\int_0^1 \sin \pi x \, dx$

e) $\int_0^{2\pi} x \sin x \, dx$

2. Use the Romberg integration procedure to find an approximation to $\int_1^3 e^x \sin x \, dx$ that is accurate within $10^{-6}$. Compare your answers to the exact result and to the result obtained in Exercise 3 of Section 4.4.

3. Use the Romberg integration procedure to find approximations to $\int_0^2 (1 + x)^{-1} \, dx$, completing the table for $n = 6$. Compare this result with the values obtained in Exercise 6 of Section 4.4 and Exercise 10 of Section 4.3.

4. Approximate $\int_1^4 \ln x \, dx$ using the Romberg integration procedure with $n = 10$.

5. Let $N = 10$. Apply the Romberg integration procedure to the integral $\int_a^b f(x) \, dx$ until $|R_{k,k} - R_{k-1,k-1}| \leq 10^{-5}$ or until $k > N$ for the following functions and values of $a$ and $b$.
   
   a) $f(x) = x^{1/3}$, $a = 0$, $b = 1$;
   
   b) $f(x) = 1.001 + .03(x - .1)^2 + 2(x - .1)^3$, $1 < x < .2$;
   
   c) $f(x) = 1.009 + .15(x - .2) + .9(x - .2)^2 + 2(x - .2)^3$, $2 < x < .3$,

   with $a = 0$, $b = .3$.

6. Show that the approximation obtained from $R_{k,2}$ is the same as that given by the Simpson's composite rule described in Theorem 4.4 with $h = h_k$.

7. Show that, for any $k$,

   $$\sum_{i=1}^{2^{k-1}-1} f\left(a + \frac{i}{2} h_{k-1}\right) = \sum_{i=1}^{2^{k-3}} f\left(a + \left(i - \frac{1}{2}\right)h_{k-1}\right) + \sum_{i=1}^{2^{k-3}-1} f\left(a + ih_{k-1}\right).$$

8. Use the result of Exercise 7 to verify Eq. (4.58); that is, show that, for all $k$,

   $$R_{k,1} = \frac{1}{2} \left[ R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f\left(a + \left(i - \frac{1}{2}\right)h_{k-1}\right) \right].$$

9. Compute an approximation to $\int_0^{2\pi} \sqrt{1 + (\cos x)^2} \, dx$ that is accurate to within $10^{-4}$ by using Romberg integration.

### 4.7 Gaussian Quadrature

The closed Newton–Cotes formulas presented in Section 4.3 were derived by integrating the Lagrange interpolating polynomials. Since the error term in the Lagrange interpolating polynomial of degree $n$ involves the $(n + 1)$st derivative of the function being approximated, it has been remarked previously that the formula is exact when approximating any polynomial of degree less than or equal to $n$. Consequently, the closed Newton–Cotes formulas have degree of precision at least $n$. In fact, the degree of precision of the odd formulas is exactly $n$, while the even formulas have degree of precision $(n + 1)$. An analogous situation occurs for the open Newton–Cotes formulas.

* This section requires some material concerning orthogonal functions, which is discussed in Section 7.2.