The exact solution:
\[ \int_{0}^{4} e^{x} \, dx = e^{4} - e^{0} = 53.59815 \]
Simpson’s Rule with \( h = 2 \)
\[ \int_{0}^{4} e^{x} \, dx \approx \frac{2}{3} (e^{0} + 4e^{2} + e^{4}) = 56.76958. \]
The error is \(-3.17143\) (5.92%).
Divide-and-Conquer: Simpson’s Rule with \( h = 1 \)
\[ \int_{0}^{2} e^{x} \, dx + \int_{2}^{4} e^{x} \, dx \approx \frac{1}{3} (e^{0} + 4e^{1} + e^{2}) + \frac{1}{3} (e^{2} + 4e^{3} + e^{4}) = 53.86385 \]
The error is \(-0.26570\). (0.50%) Improvement by a factor of 10!
Divide and Conquer with Simpson’s Rule

Extending the table...

<table>
<thead>
<tr>
<th>$h$</th>
<th>abs-error</th>
<th>err/h</th>
<th>err/h²</th>
<th>err/h³</th>
<th>err/h⁴</th>
<th>err/h⁵</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3.171433</td>
<td>1.585716</td>
<td>0.792858</td>
<td>0.396429</td>
<td>0.198215</td>
<td>0.099107</td>
</tr>
<tr>
<td>1</td>
<td>0.265696</td>
<td>0.265696</td>
<td>0.265696</td>
<td>0.265696</td>
<td>0.265696</td>
<td>0.265696</td>
</tr>
<tr>
<td>1/2</td>
<td>0.018071</td>
<td>0.036142</td>
<td>0.072283</td>
<td>0.144566</td>
<td>0.289132</td>
<td>0.578264</td>
</tr>
<tr>
<td>1/4</td>
<td>0.001155</td>
<td>0.004618</td>
<td>0.018473</td>
<td>0.073892</td>
<td>0.295566</td>
<td>1.182266</td>
</tr>
<tr>
<td>1/8</td>
<td>0.000073</td>
<td>0.000580</td>
<td>0.004644</td>
<td>0.037152</td>
<td>0.297215</td>
<td>2.377716</td>
</tr>
</tbody>
</table>

Clearly, the err/h⁴ column seems to converge (to a non-zero constant) as $h \rightarrow 0$. The columns to the left seem to converge to zero, and the err/h⁵ column seems to grow.

This is numerical evidence that the composite Simpson’s rule has a convergence rate of $O(h^4)$. But, isn’t Simpson’s rule 5th order???

Generalized Composite Simpson’s Rule

For an even integer $n$: Subdivide the interval $[a, b]$ into $n$ subintervals, and apply Simpson’s rule on each consecutive pair of sub-intervals. With $h = (b - a)/n$ and $x_j = a + jh$, $j = 0, 1, \ldots, n$, we have

$$
\int_a^b f(x)dx = \frac{h}{3} \left[ f(x_0) - f(x_n) + \sum_{j=1}^{n/2} [4f(x_{2j-1}) + 2f(x_{2j})] \right]
- \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j).
$$

The error term is:

$$
E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j), \quad \xi_j \in [x_{2j-2}, x_{2j}]
$$

The Error for Composite Simpson’s Rule

If $f \in C^4[a, b]$, the Extreme Value Theorem implies that $f^{(4)}$ assumes its max and min in $[a, b]$. Now, since

$$
\min_{x \in [a, b]} f^{(4)}(x) \leq \frac{n}{2} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \max_{x \in [a, b]} f^{(4)}(x),
$$

and

$$
\frac{n}{2} \min_{x \in [a, b]} f^{(4)}(x) \leq \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \frac{n}{2} \max_{x \in [a, b]} f^{(4)}(x),
$$

By the Intermediate Value Theorem $\exists \mu \in (a, b)$ so that

$$
f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \iff \frac{n}{2} f^{(4)}(\mu) = \sum_{j=1}^{n/2} f^{(4)}(\xi_j)
$$
We can now rewrite the error term:

\[ E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu), \]

or, since \( h = (b - a)/n \) \( \Leftrightarrow \) \( n = (b - a)/h \), we can write

\[ E(f) = -\frac{(b - a)}{180} h^4 f^{(4)}(\mu). \]

Hence **Composite Simpson’s Rule** has **degree of accuracy 3** (since it is exact for polynomials up to order 3), and the error is proportional to \( h^4 \) — **Convergence Rate** \( O(h^4) \).

---

**Algorithm (Composite Simpson’s Rule)**

Given the end points \( a \) and \( b \) and an even positive integer \( n \):

1. \( h = (b - a)/n \)
2. \( ENDPTS = f(a) + f(b) \)
   - \( ODDPTS = 0 \)
   - \( EVENPTS = 0 \)
3. FOR \( i = 1, \ldots, n-1 \) — (interior points)
   - \( x = a + i \cdot h \)
   - if \( i \) is even: \( EVENPTS += f(x) \)
   - if \( i \) is odd: \( ODDPTS += f(x) \)
   - END
4. \( INTAPPROX = h \cdot (ENDPTS + 2 \cdot EVENPTS + 4 \cdot ODDPTS) / 3 \)

---

Homework #7 — Due Friday 11/13/2009, 12-noon

(Part-1)

Implement Composite Simpson’s Rule, and use your code to solve BF-4.4.3-a,b,c,d.

---

**Romberg Integration**

**The Return of Richardson’s Extrapolation**

**Romberg Integration** is the combination of the **Composite Trapezoidal Rule** (CTR)

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

and **Richardson Extrapolation**.

Here, we know that the error term for regular Trapezoidal Rule is \( O(h^3) \). By the same argument as for Composite Simpson’s Rule, this gets reduced to \( O(h^2) \) for the composite version.
Romberg Integration

Step-1: CTR Refinement

Let $R_{k,1}$ denote the Composite Trapezoidal Rule with $2^{k-1}$ sub-intervals, and $h_k = (b - a)/2^{k-1}$. We get:

$$
R_{1,1} = \frac{h_1}{2} [f(a) + f(b)] \\
R_{2,1} = \frac{h_2}{2} [f(a) + 2f(a + h_2) + f(b)] \\
= \frac{(b-a)}{4} [f(a) + f(b) + 2f(a + h_2)] \\
= \frac{1}{2} [R_{1,1} + h_1 f(a + h_2)] \\
\vdots \\
R_{k,1} = \frac{1}{2} \left[ R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k) \right]
$$

Update formula, using previous value + new points

Extrapolate using Richardson

We know that the error term is $O(h^2)$, so in order to eliminate this term we combine to consecutive entries $R_{k-1,1}$ and $R_{k,1}$ to form a higher order approximation $R_{k,2}$ of the integral.

$$
R_{k,2} = R_{k,1} + \frac{R_{k,1} - R_{k-1,1}}{2^2 - 1}
$$

<table>
<thead>
<tr>
<th>$k$</th>
<th>$R_{k,1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1.5707963267949</td>
</tr>
<tr>
<td>3</td>
<td>1.8961188979370</td>
</tr>
<tr>
<td>4</td>
<td>1.9742316019455</td>
</tr>
<tr>
<td>5</td>
<td>1.9935703437723</td>
</tr>
<tr>
<td>6</td>
<td>1.9963933609701</td>
</tr>
<tr>
<td>7</td>
<td>1.9999983886400</td>
</tr>
</tbody>
</table>

Extrapolate, again...

It turns out (Taylor expand to check) that the complete error term for the Trapezoidal rule only has even powers of $h$:

$$
\int_a^b f(x) = R_{k,1} - \sum_{i=1}^{\infty} E_{2i} h_k^{2i}.
$$

Hence the $R_{k,2}$ approximations have error terms that are of size $O(h^4)$.

To get $O(h^6)$ approximations, we compute

$$
R_{k,3} = R_{k,2} + \frac{R_{k,2} - R_{k-1,2}}{4^2 - 1}
$$
Extrapolate, yet again...

In general, since we only have even powers of $h$ in the error expansion:

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$

Revisiting $\int_0^\pi \sin(x) dx$:

<table>
<thead>
<tr>
<th>$R_{k,1}$ — $O(h^2)$</th>
<th>$R_{k,2}$ — $O(h^3)$</th>
<th>$R_{k,3}$ — $O(h^4)$</th>
<th>$R_{k,4}$ — $O(h^5)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.570796326794897</td>
<td>2.094395102393195</td>
<td>1.998570731823836</td>
<td>1.974231601945551</td>
</tr>
<tr>
<td>1.896118897937040</td>
<td>2.004559754984421</td>
<td>2.004559754984421</td>
<td>2.004559754984421</td>
</tr>
<tr>
<td>1.974231601945551</td>
<td>2.004559754984421</td>
<td>2.004559754984421</td>
<td>2.004559754984421</td>
</tr>
<tr>
<td>1.999999996190846</td>
<td>2.000000000000000</td>
<td>2.000000000000000</td>
<td>2.000000000000000</td>
</tr>
</tbody>
</table>

Homework? No, enough already — Here's the code outline!

Code (Romberg Quadrature)

```matlab
% Romberg Integration for sin(x) over [0,pi]
a = 0; b = pi; % The Endpoints
R = zeros(7,7);
R(1,1) = (b - a)/2 * (sin(a) + sin(b));
for k = 2 : 7
    h = (b - a)/(2^(k-1));
    R(k,1)=1/2 * (R(k-1,1) + 2 * h * sum(sin(a + 2 * (1 : (2^(k-2))) - 1) * h));
end
for j = 2 : 7
    for k = j : 7
        R(k,j) = R(k,j-1) + (R(k,j-1) - R(k-1,j-1))/(4^(j-1));
    end
end
disp(R)
```

More Advanced Numerical Integration Ideas

Adaptive and Gaussian Quadrature

The composite formulas require equally spaced nodes.

This is not good if the function we are trying to integrate has both regions with large fluctuations, and regions with small variations.

We need many points where the function fluctuates, but few points where it is close to constant or linear.
**Introduction — Adaptive Quadrature Methods**

**Idea** Cleverly predict (or measure) the amount of variation and automatically add more points where needed.

We are going to discuss this in the context of Composite Simpson’s rule, but the approach can be adopted for other integration schemes.

**First** we are going to develop a way to measure the error — a numerical estimate of the actual error in the numerical integration. Note: just knowing the structure of the error term is not enough! (We will however use the structure of the error term in our derivation of the numerical error estimate.)

**Then** we will use the error estimate to decide whether to accept the value from CSR, or if we need to refine further (recompute with smaller $h$).

---

**Composite Simpson’s Rule (CSR)**

With this notation, we can write CSR with $n = 4$, and $h_2 = (b - a)/4 = h_1/2$:

$$
\int_a^b f(x) \, dx = S(f; a, b) = S(f; a, \frac{a+b}{2}) + S(f; \frac{a+b}{2}, b) - E(f; h_2, \mu_2).
$$

We can squeeze out an estimate for the error by noticing that

$$
E(f; h_2, \mu_2) = \frac{1}{16} \left( \frac{h_1^5}{90} f^{(4)}(\mu_1) \right) = \frac{1}{16} E(f; h_1, \mu_2).
$$

Now, assuming $f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2)$, we do a little bit of algebra magic with our two approximations to the integral...

---

**Some Notation — One-step Simpson’s Rule**

**Notation — “One-step” Simpson’s Rule:**

$$
\int_a^b f(x) \, dx = S(f; a, b) - \frac{h_1^5}{90} f^{(4)}(\mu_1), \quad \mu_1 \in (a, b),
$$

where

$$
S(f; a, b) = \frac{b-a}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right], \quad h_1 = \frac{b-a}{2}.
$$

---

**Wait! Wait! Wait! — I pulled a fast one!**

$$
E(f; h_2, \mu_2) = \frac{1}{32} \left( \frac{h_1^5}{90} f^{(4)}(\mu_1) \right) + \frac{1}{32} \left( \frac{h_2^5}{90} f^{(4)}(\mu_2) \right)
$$

where $\mu_1 \in [a, \frac{a+b}{2}]$, $\mu_2 \in [\frac{a+b}{2}, b]$.

If $f \in C^4[a, b]$, then we can use our old friend, the intermediate value theorem:

$$
\exists \mu_2 \in [\mu_1^1, \mu_2^2] \subset [a, b]: \quad f^{(4)}(\mu_2) = \frac{f^{(4)}(\mu_1^1) + f^{(4)}(\mu_2^2)}{2}.
$$

So it follows that

$$
E(f; h_2, \mu_2) = \frac{1}{16} \left( \frac{h_1^5}{90} f^{(4)}(\mu_2) \right).
$$
Back to the Error Estimate...

Now we have

\[
S(f; a, a+b/2) + S(f; a+b/2, b) - \frac{1}{16} \left( \frac{h^5}{90} f^{(4)}(\mu_2) \right) = S(f; a, b) - \frac{h^5}{90} f^{(4)}(\mu_1).
\]

Now use the assumption \( f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2) \) (and replace \( \mu_1 \) and \( \mu_2 \) by \( \mu \)):

\[
\frac{h^5}{90} f^{(4)}(\mu) \approx \frac{16}{15} S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b),
\]

notice that \( \frac{h^5}{90} f^{(4)}(\mu) = E(f; h_1, \mu) = 16E(f; h_2, \mu) \). Hence

\[
E(f; h_2, \mu) \approx \frac{1}{15} S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b),
\]

Putting it Together...

Finally, we have the error estimate in hand...

Using the estimate of \( \frac{h^5}{90} f^{(4)}(\mu) \), we have

\[
\int_a^b f(x) dx - S(f; a, (a+b)/2) - S(f; (a+b)/2, b) \approx \frac{1}{15} S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b)
\]

Notice!!! \( S(f; a, (a+b)/2) + S(f; (a+b)/2, b) \) approximates \( \int_a^b f(x) dx \) **15 times better** than it agrees with the known quantity \( S(f; a, b) \)!!!
Adaptive Quadrature

We want to approximate \( \int_a^b f(x) \, dx \) with an error less than \( \epsilon \) (a specified tolerance).

[1] Compute the two approximations
\[
S_1(f(x); a, b) = S(f(x); a, b),
\]
and
\[
S_2(f(x); a, b) = S(f(x); a, \frac{a+b}{2}) + S(f(x); \frac{a+b}{2}, b).
\]

[2] Estimate the error, if the estimate is less than \( \epsilon \), we are done. Otherwise...

[3] Apply steps [1] and [2] recursively to the intervals \([a, \frac{a+b}{2}]\) and \([\frac{a+b}{2}, b]\) with tolerance \(\epsilon/2\).

Adaptive Quadrature, Interval Refinement Example #1

The funny figure above is supposed to illustrate a possible sub-interval refinement hierarchy. Red dashed lines illustrate failure to satisfy the tolerance, and black lines illustrate satisfied tolerance.

<table>
<thead>
<tr>
<th>level</th>
<th>tol</th>
<th>interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(\epsilon)</td>
<td>([a, b])</td>
</tr>
<tr>
<td>2</td>
<td>(\epsilon/2)</td>
<td>([a, a + \frac{b-a}{2}])</td>
</tr>
<tr>
<td>3</td>
<td>(\epsilon/4)</td>
<td>([a, a + \frac{b-a}{4}])</td>
</tr>
<tr>
<td></td>
<td></td>
<td>\vdots</td>
</tr>
</tbody>
</table>

Gaussian Quadrature

Idea: Evaluate the function at a set of optimally chosen points in the interval.

We will choose \(\{x_0, x_1, \ldots, x_n\} \in [a, b]\) and coefficients \(c_i\), so that the approximation
\[
\int_a^b f(x) \, dx \approx \sum_{i=0}^n c_i f(x_i)
\]
is exact for the largest class of polynomials possible.

We have already seen that the open Newton-Cotes formulas sometimes give us better “bang-for-buck” than the closed formulas (e.g. the mid-point formula uses only 1 point and is as accurate as the two-point trapezoidal rule). — Gaussian quadrature takes this one step further.
Higher Order Gaussian Quadrature Formulas

We could obtain higher order formulas by adding more points, computing the integrals, and solving the resulting non-linear system of equations... but it gets very painful, very fast.

The Legendre Polynomials come to our rescue!

The Legendre polynomials $P_n(x)$ are orthogonal on $[-1,1]$ with respect to the weight function $w(x) = 1$, i.e.

$$\int_{-1}^{1} P_n(x) P_m(x) \, dx = \alpha_n \delta_{n,m} = \begin{cases} 0 & m \neq n \\ \alpha_n & m = n \end{cases}$$

if $P(x)$ is a polynomial of degree less than $n$, then

$$\int_{-1}^{1} P_n(x) P(x) \, dx = 0.$$

A Quick Note on Legendre Polynomials

We will see Legendre polynomials in more detail later. For now, all we need to know is that they satisfy the property

$$\int_{-1}^{1} P_n(x) P_m(x) \, dx = \alpha_n \delta_{n,m}.$$

and the first few Legendre polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = x^2 - 1/3, \quad P_3(x) = x^3 - 3x/5, \quad P_4(x) = x^4 - 6x^2/7 + 3/35, \quad P_5(x) = x^5 - 10x^3/9 + 5x/21.$$  

It turns out that the roots of the Legendre polynomials are the nodes in Gaussian quadrature.
Higher Order Gaussian Quadrature Formulas

**Proof of the Theorem**

Let us first consider a polynomial, $P(x)$ with degree less than $n$. $P(x)$ can be rewritten as an $(n-1)$-st Lagrange polynomial with nodes at the roots of the $n^{th}$ Legendre polynomial $P_n(x)$. This representation is exact since the error term involves the $n^{th}$ derivative of $P(x)$, which is zero. Hence,

$$\int_{-1}^{1} P(x) \, dx = \int_{-1}^{1} \left[ \sum_{i=1}^{n} \prod_{j=1 \atop j \neq i}^{n} \frac{x - x_j}{x_i - x_j} P(x_j) \right] \, dx$$

$$= \sum_{i=1}^{n} \left[ \int_{-1}^{1} \prod_{j=1 \atop j \neq i}^{n} \frac{x - x_j}{x_i - x_j} \, dx \right] P(x_j) = \sum_{i=1}^{n} c_i P(x_i),$$

which verifies the result for polynomials of degree less than $n$.

---

If the polynomial $P(x)$ of degree $[n,2n)$ is divided by the $n^{th}$ Legendre polynomial $P_n(x)$, we get:

$$P(x) = Q(x)P_n(x) + R(x)$$

where both $Q(x)$ and $R(x)$ are of degree less than $n$.

[1] Since $\deg(Q(x)) < n$

$$\int_{-1}^{1} Q(x)P_n(x) \, dx = 0.$$

[2] Further, since $x_i$ is a root of $P_n(x)$:

$$P(x_i) = Q(x_i)P_n(x_i) + R(x_i) = R(x_i).$$

[3] Now, since $\deg(R(x)) < n$, the first part of the proof implies

$$\int_{-1}^{1} R(x) \, dx = \sum_{i=1}^{n} c_i R(x_i).$$

Putting [1], [2] and [3] together we arrive at

$$\int_{-1}^{1} P(x) \, dx = \int_{-1}^{1} [Q(x)P_n(x) + R(x)] \, dx$$

$$= \int_{-1}^{1} R(x) \, dx + \sum_{i=1}^{n} c_i R(x_i)$$

$$= \sum_{i=1}^{n} c_i P(x_i),$$

which shows that the formula is exact for all polynomials $P(x)$ of degree less than $2n$. □
Gaussian Quadrature beyond the interval \([-1, 1]\)

By a simple linear transformation,
\[
t = \frac{2x - a - b}{b - a} \quad \Rightarrow \quad x = \frac{(b - a)t + (b + a)}{2},
\]
we can apply the Gaussian Quadrature formulas to any interval
\[
\int_a^b f(x) \, dx = \int_{-1}^1 f \left( \frac{(b - a)t + (b + a)}{2} \right) \frac{(b - a)}{2} \, dt.
\]

Examples

\[
\int_0^{\pi/4} (\cos(x))^2 \, dx = \frac{1}{4} + \frac{\pi}{8} = 0.642699081698724
\]

<table>
<thead>
<tr>
<th>Degree</th>
<th>Quadrature points</th>
<th>Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.16597, 0.61942</td>
<td>1, 1</td>
</tr>
<tr>
<td>3</td>
<td>0.08851, 0.39270, 0.69688</td>
<td>0.55556, 0.88889, 0.55556</td>
</tr>
<tr>
<td>4</td>
<td>0.05453, 0.25919, 0.52621, 0.73087</td>
<td>0.34785, 0.65215, 0.65215, 0.34785</td>
</tr>
</tbody>
</table>

Table: Quadrature points translated to interval of interest; with weight coefficients.

\[
\begin{array}{c|c|c}
\text{Degree} & \text{Integral approximation} & \text{Error} \\
\hline
2 & 0.642317235049753 & 0.0003818466489... \\
3 & 0.642701112090729 & 0.0000002030920... \\
4 & 0.642699075999924 & 0.0000000056988... \\
\end{array}
\]

Table: Approximation and Error, for GQ.