Numerical Integration

Consider the integral $\int_0^\pi \frac{\sin x}{x} \, dx$. How can we evaluate this?

The antiderivative of $\frac{\sin x}{x}$ is not an elementary function so we cannot use the Fundamental Theorem of calculus. How can we proceed?

We can at least approximate. Recall Riemann Sums.

**Left hand sum** \( \text{LEFT} = \sum_{i=0}^{n-1} f(x_i) \Delta x \)

**Right hand sum** \( \text{RIGHT} = \sum_{i=0}^{n-1} f(x_{i+1}) \Delta x \)

**Midpoint sum** \( \text{MID} = \sum_{i=0}^{n-1} f\left(\frac{x_i + x_{i+1}}{2}\right) \Delta x \)

where \( \Delta x = \frac{b-a}{n} \) and \( a = x_0, \ b = x_n \)
Numerical Integration

Which of these do you think is the most accurate?

(midpoint)

Suppose \( f(x) \) is strictly decreasing on \([a, b] \). Then

a) LEFT is an (over/under) estimate

b) RIGHT is an (over/under) estimate

Repeat for strictly increasing \( f(x) \).

Errors

Consider \( I = \int_0^4 (x+1)e^x \, dx \). This is difficult to do [at least now] until you notice that

if \( F(x) = xe^x \) then \( F'(x) = f(x) = (x+1)e^x \)

\[ I = xe^x \bigg|_0^4 = 4e^4 - 0 \approx 218.392600 \]

If we try LEFT and RIGHT with \( n = 2 \) we find

\[
\text{LEFT} = f(x_0) \Delta x + f(x_1) \Delta x; \quad \Delta x = \frac{4-0}{2} = 2
\]

\[ = (0+1)e^0 \cdot 2 + (2+1)e^2 \cdot 2 \]

\[ = 2 + 44.33433366 \]

\[ \text{Error} = I - \text{LEFT} \]

\[ = 46.33433366 \]

\[ \approx 172.05826 \]

\[
\text{RIGHT} = f(x_1) \Delta x + f(x_2) \Delta x
\]

\[ = 2 \left[ (2+1)e^2 + (4+1)e^4 \right] \]

\[ \text{Error} = I - \text{RIGHT} \]

\[ = 590.3158369 \]

\[ \approx -371.92324 \]
Numerical Integration

These answers are not very good estimates, so the errors are quite large.

We should be able to reduce the error, however, by increasing the number of intervals.

(Show overhead for Left & Right Hand Sums)

What is most interesting here is that when the number of intervals is doubled, the error is reduced (as \( n \to \infty \)) by a factor of 2.

Can we do better? Yes!

1) We expect the midpoint rule will do better
2) the average of LEFT and RIGHT should be better \( \Rightarrow \) Trapezoid Rule (TRAP).

\[
TRAP = \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2} \Delta x
\]

\[
\text{Area} = \frac{f(x_i) + f(x_{i+1})}{2} \Delta x
\]

\[\Delta x = x_{i+1} - x_i\]
Errors obtained by Left and Right Hand Sums of 
\[ \int_{0}^{4} (x + 1)e^x \, dx \]
as the number of intervals \( n \) is increased.

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \text{**** LEFT HAND RULE ***} )</th>
<th>( \text{**** RIGHT HAND RULE ***} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>\text{error}</td>
<td>\text{ratio}</td>
</tr>
<tr>
<td>1</td>
<td>214.3926001326</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>172.0582635390</td>
<td>1.25</td>
</tr>
<tr>
<td>4</td>
<td>109.4467204861</td>
<td>1.57</td>
</tr>
<tr>
<td>8</td>
<td>61.2518766801</td>
<td>1.79</td>
</tr>
<tr>
<td>16</td>
<td>32.3054119075</td>
<td>1.90</td>
</tr>
<tr>
<td>32</td>
<td>16.5756246874</td>
<td>1.95</td>
</tr>
<tr>
<td>64</td>
<td>8.3937341434</td>
<td>1.97</td>
</tr>
<tr>
<td>128</td>
<td>4.2233595520</td>
<td>1.99</td>
</tr>
<tr>
<td>256</td>
<td>2.1183036484</td>
<td>1.99</td>
</tr>
<tr>
<td>512</td>
<td>1.0608078393</td>
<td>2.00</td>
</tr>
<tr>
<td>1024</td>
<td>0.5308179264</td>
<td>2.00</td>
</tr>
</tbody>
</table>
Numerical Integration

This is just the average of LEFT and RIGHT:

\[
\frac{1}{2} (\text{LEFT} + \text{RIGHT}) = \frac{1}{2} \left[ \sum_{i=0}^{n-1} f(x_i) \Delta x + \sum_{i=0}^{n-1} f(x_{i+1}) \Delta x \right]
\]

\[
= \frac{1}{2} \sum_{i=0}^{n-1} (f(x_i) + f(x_{i+1})) \Delta x
\]

\[
= \sum_{i=0}^{n-1} \frac{f(x_i) + f(x_{i+1})}{2} \Delta x
\]

(Show overhead for Midpoint & Trapezoid Rules)

1) Errors reduce by factor of 4 when the # of intervals increase by factor of 2.
2) Errors for MID are about half the size of errors for TRAP.

Question: If \( f(x) \) is concave up, will MID overestimate or underestimate the correct value? (under)

Repeat for TRAP. (overestimator)

Repeat for case when \( f(x) \) is concave down.

So 1) MID overestimates when TRAP underestimates and vice-versa.
2) Errors from MID are twice as small as TRAP's errors.
Errors obtained by Midpoint and Trapezoid Rules applied to
\[ \int_0^4 (x + 1) e^x \, dx \]
as the number of intervals \( n \) is increased.

<table>
<thead>
<tr>
<th>( n )</th>
<th><strong>MIDPOINT RULE</strong></th>
<th>( \text{ratio} )</th>
<th><strong>TRAPEZOID RULE</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>error</strong></td>
<td><strong>ratio</strong></td>
<td><strong>error</strong></td>
</tr>
<tr>
<td>1</td>
<td>129.7239269454</td>
<td>2.77</td>
<td>-329.5889001989</td>
</tr>
<tr>
<td>2</td>
<td>46.8351774332</td>
<td>3.59</td>
<td>-99.9324866267</td>
</tr>
<tr>
<td>4</td>
<td>13.0570328741</td>
<td>3.89</td>
<td>-26.5486545967</td>
</tr>
<tr>
<td>8</td>
<td>3.3589471348</td>
<td>3.97</td>
<td>-6.7458108613</td>
</tr>
<tr>
<td>16</td>
<td>0.8458374674</td>
<td>3.99</td>
<td>-1.6934318632</td>
</tr>
<tr>
<td>32</td>
<td>0.2118435994</td>
<td>4.00</td>
<td>-0.4237971979</td>
</tr>
<tr>
<td>64</td>
<td>0.0529849607</td>
<td>4.00</td>
<td>-0.1059767993</td>
</tr>
<tr>
<td>128</td>
<td>0.0132477447</td>
<td>4.00</td>
<td>-0.0264959193</td>
</tr>
<tr>
<td>256</td>
<td>0.0033120302</td>
<td>4.00</td>
<td>-0.0066240873</td>
</tr>
<tr>
<td>512</td>
<td>0.0008280134</td>
<td>4.00</td>
<td>-0.0016560285</td>
</tr>
<tr>
<td>1024</td>
<td>0.0002070037</td>
<td>4.00</td>
<td>-0.0004140076</td>
</tr>
</tbody>
</table>
Can we combine these rules (like we did with LEFT and RIGHT) to get a more accurate rule? How?

Try weighted average: \[
\frac{2 \text{ MID} + \text{TRAP}}{3}
\]

This is called **Simpson's Rule**. It does much better than any rule we've seen yet.

(Show overhead for Simpson's Rule)

Notice that when \( n \) is increased by a factor of 2, the error is reduced by a factor of 16.

**Trapezoid & Simpson's Rule for \( \int_a^b f(x) \, dx \)**

\[
\text{TRAP} = \sum_{i=0}^{n-1} \left( \frac{f(x_i) + f(x_{i+1})}{2} \right) \Delta x
\]

\[
= \frac{\Delta x}{2} \left[ f(x_0) + f(x_1) + f(x_2) + \ldots + f(x_{n-2}) + f(x_{n-1}) + f(x_n) \right]
\]

\[
= \frac{\Delta x}{2} \left[ f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n) \right]
\]

and since \( \frac{b-a}{n} = \Delta x \)

\[
\text{TRAP} = \frac{b-a}{2n} \left[ f(x_0) + 2f(x_1) + 2f(x_2) + \ldots + 2f(x_{n-1}) + f(x_n) \right]
\]

where \( a = x_0, \ b = x_n \)

This is the composite Trapezoid rule.

Integrates linear functions exactly.
Errors obtained by Simpson’s Rule applied to \( \int_0^4 (x + 1)e^x \, dx \) as the number of intervals \( n \) is increased.

<table>
<thead>
<tr>
<th>n</th>
<th>error</th>
<th>ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-23.3803487693</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-2.0873772534</td>
<td>11.20</td>
</tr>
<tr>
<td>4</td>
<td>-0.1448629495</td>
<td>14.41</td>
</tr>
<tr>
<td>8</td>
<td>-0.0093055305</td>
<td>15.57</td>
</tr>
<tr>
<td>16</td>
<td>-0.0005856428</td>
<td>15.89</td>
</tr>
<tr>
<td>32</td>
<td>-0.0000366664</td>
<td>15.97</td>
</tr>
<tr>
<td>64</td>
<td>-0.000022926</td>
<td>15.99</td>
</tr>
<tr>
<td>128</td>
<td>-0.000001433</td>
<td>16.00</td>
</tr>
<tr>
<td>256</td>
<td>-0.000000090</td>
<td>16.00</td>
</tr>
<tr>
<td>512</td>
<td>-0.000000006</td>
<td>16.00</td>
</tr>
<tr>
<td>1024</td>
<td>-0.0000000000000</td>
<td>15.99</td>
</tr>
</tbody>
</table>
Numerical Integration

The trapezoid rule integrates linear functions exactly because the trapezoids fit exactly between any straight line and the horizontal axis.

Polynomials are easy to integrate, so perhaps we could find a way to approximate \( \int_a^b f(x) \, dx \) by approximating \( f(x) \) using polynomials and then integrating those.

If we use polynomials of degree 1 we have the Trapezoid Rule. Let's try quadratics...

\[
\begin{align*}
f(x_i) &= p(x_i), \
f(x_i+1) &= p(x_{i+1}), \
f(x_{i+2}) &= p(x_{i+2})
\end{align*}
\]

Take points in groups of 3, overlapping at endpoints, and find parabola \( p(x) = Ax^2 + Bx + C \) that fits these points, i.e.

and note that \( x_{i+1} = \frac{x_i + x_{i+2}}{2} \) (midpoint) when the points are equally spaced.
Numerical Integration

It can be shown (see next sheet 7a) that

\[
\int_{x_i}^{x_{i+2}} p(x) \, dx = \frac{h}{3} \left[ p(x_i) + 4p(x_{i+1}) + p(x_{i+2}) \right]
\]

where \( h = \frac{x_{i+2} - x_i}{2} \) (spacing)

but then

\[
\int_{x_i}^{x_{in}} f(x) \, dx \approx \frac{h}{3} \left[ f(x_i) + 4f(x_{i+1}) + f(x_{i+2}) \right]
\]

This is Simpson's Rule for 3 points. If we want more intervals we do

\[
\int_{x_0}^{x_n} f(x) \, dx \approx \frac{h}{3} \left[ f(x_0) + 4f(x_1) + 2f(x_2) + \cdots + 4f(x_{n-1}) + f(x_n) \right]
\]

\[
= \frac{b-a}{3n} \left[ f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \right]
\]

\[
\text{Simp} = \frac{b-a}{3n} \left[ f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \right]
\]

where \( a = x_0, \ b = x_n \)

This is the composite Simpson's Rule.
Let \( p(x) = Ax^2 + Bx + C \) and let \( x_1 = (x_0 + x_2)/2 \) be the midpoint of \([x_0, x_2]\).

\[
\int_{x_0}^{x_2} Ax^2 + Bx + C \, dx = \left. \frac{A}{3} x^3 + \frac{B}{2} x^2 + Cx \right|_{x_0}^{x_2}
\]
\[
= \frac{A}{3} x_2^3 + \frac{B}{2} x_2^2 + Cx_2 - \frac{A}{3} x_0^3 + \frac{B}{2} x_0^2 + Cx_0
\]
\[
= \frac{A}{3} (x_2^3 - x_0^3) + \frac{B}{2} (x_2^2 - x_0^2) + C(x_2 - x_0)
\]
\[
= \frac{A}{3} (x_2 - x_0)(x_2^2 + x_2x_0 + x_0^2) + \frac{B}{2} (x_2 - x_0)(x_2 + x_0) + C(x_2 - x_0)
\]
\[
= \frac{x_2 - x_0}{6} \left[ 2A(x_2^2 + x_2x_0 + x_0^2) + 3B(x_2 + x_0) + 6C \right]
\]
\[
= \frac{x_2 - x_0}{6} \left[ Ax_2^2 + Bx_2 + C + Ax_0^2 + Bx_0 + C + A(x_2^2 + 2x_2x_0 + x_0^2) + 2B(x_2 + x_0) + 4C \right]
\]
\[
= \frac{x_2 - x_0}{6} \left[ (Ax_2^2 + Bx_2 + C) + (Ax_0^2 + Bx_0 + C) + 4A \left( \frac{x_2 + x_0}{2} \right)^2 \right] + 4B \frac{x_2 + x_0}{2} + 4C
\]
\[
= \frac{x_2 - x_0}{6} \left[ p(x_2) + p(x_0) + 4 \left( A \left( \frac{x_2 + x_0}{2} \right)^2 \right) + B \left( \frac{x_2 + x_0}{2} \right) + C \right]
\]
\[
= \frac{x_2 - x_0}{6} \left[ p(x_2) + p(x_0) + 4 \left( Ax_1^2 + Bx_1 + C \right) \right]
\]
\[
= \frac{x_2 - x_0}{6} \left[ p(x_0) + 4p(x_1) + p(x_2) \right]
\]

If \( h = x_1 - x_0 = x_2 - x_1 \) is the spacing then the formula reduces to

\[
\int_{x_0}^{x_2} p(x) \, dx = \frac{h}{3} \left[ p(x_0) + 4p(x_1) + p(x_2) \right]
\]
Numerical Integration

Ex \[ \int_{0}^{1} \cos x \, dx \]

Exact answer \[ \int_{0}^{1} \cos x \, dx = \sin x \bigg|_{0}^{1} = \sin 1 \approx 0.84147 \]

Midpoint Rule with \( n = 4 \)

\[
\text{MID} = \frac{1}{4} \left[ \cos (0.125) + \cos (0.375) + \cos (0.625) + \cos (0.875) \right]
\]
\[
= 0.84267
\]

Trapezoidal Rule with \( n = 4 \)

\[
\text{TRAP} = \frac{1}{8} \left[ \cos (0) + 2 \cos (0.25) + 2 \cos (0.5) + 2 \cos (0.75) + \cos (1.0) \right]
\]
\[
= 0.83708
\]

Simpson's Rule

\[
\text{Simp} = \frac{1}{12} \left[ \cos (0) + 4 \cos (0.25) + 2 \cos (0.5) + 4 \cos (0.75) + \cos (1.0) \right]
\]
\[
= 0.84149
\]
Numerical Integration

Errors

Suppose \( f'' \) is continuous on \([a, b]\) and that
\[
|f''(x)| \leq K \text{ for all } x \text{ in } [a, b]. \text{ Then}
\]

**TRAP** \[ |ET_n| \leq K \frac{(b-a)^3}{12n^2} = K \frac{b-a}{12} (\Delta x)^2 \]

**MID** \[ |EM_n| \leq K \frac{(b-a)^3}{24n^2} = K \frac{b-a}{24} (\Delta x)^2 \]

**Ex** How many intervals are required to evaluate
\[
\int_1^2 \sin x \, dx \text{ to an accuracy of } 10^{-5}\text{ using}
\]

The Trapezoid Rule?

\[
f(x) = \sin x \text{ so } f'(x) = \cos x, \quad f''(x) = -\sin x
\]

Notice that \( \max_{[1,2]} \left| -\sin x \right| = 1 \) so we use \( K = 1 \).

Need \( |ET_n| \leq 10^{-5} \) so \[ K \frac{(b-a)^3}{12n^2} = (1) \frac{(2-1)^3}{12n^2} \leq 10^{-5} \]

\[
\frac{1}{12n^2} \leq 10^{-5}
\]
Need \( n \geq 92 \)

\[
12n^2 \geq 10^5
\]
\[
n^2 \geq \frac{10^5}{12}
\]
\[
n \geq \sqrt{\frac{10^5}{12}}
\]
\[
n \geq 91.287
\]

Using Trapezoid Rule
Numerical Integration

Thm Suppose $f^{(4)}$ is continuous on $[a, b]$ and that $|f^{(4)}(x)| \leq L$ for all $x$ in $[a, b]$. Then

$$|E_{S_n}| \leq L \frac{(b-a)^5}{180 n^4} = L \frac{b-a}{180} (\Delta x)^4$$

Ex Repeat last example using Simpson's Rule

$f(x) = \sin x \Rightarrow f^{(4)}(x) = \sin x$, $\max_{[1,2]} |\sin x| = 1$

So $L = 1$

Need $|E_{S_n}| \leq 10^{-5}$ so $(1) \frac{(2-1)^5}{180 n^4} \leq 10^{-5}$

$$180 n^4 \geq 10^5$$

$$n^4 \geq \frac{10^5}{180}$$

$$n \geq \sqrt[4]{\frac{10^5}{180}}$$

$$n \geq 4.855$$

We need $n \geq 5$ to ensure an accuracy of $10^{-5}$ using Simpson's Rule.