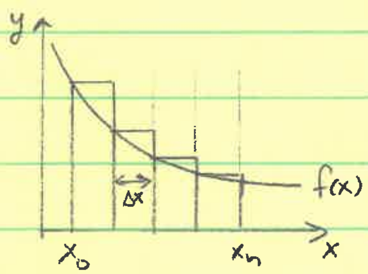
Numerical Integration

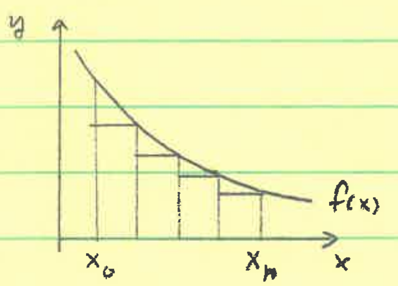
Consider the integral $\int_0^{\pi} \frac{\sin x}{x}\,dx$. How can we evaluate this?

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

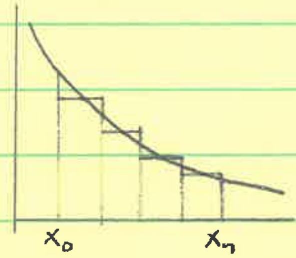
We can at least approximate. Recall Riemann Sums



left hand sum $\quad \text{LEFT} = \sum_{i=0}^{n-1} f(x_i)\,\Delta x$



right hand sum $\quad \text{RIGHT} = \sum_{i=0}^{n-1} f(x_{i+1})\,\Delta x$



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

where $\Delta x = \dfrac{b-a}{n}$ and $a = x_0$, $b = x_n$

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 $F'(x) = f(x) = (x+1)e^x$

$$\therefore \quad I = xe^x \Big|_0^4 = 4e^4 - 0 \simeq 218.392600$$

If we try LEFT and RIGHT with $n=2$ we find

$$\text{LEFT} = f(x_0)\Delta x + f(x_1)\Delta x \, ; \qquad \Delta x = \frac{4-0}{2} = 2$$

$$= (0+1)e^0 \cdot 2 + (2+1)e^2 \cdot 2$$

$$= 2 + 44.3343366 \qquad \text{Error} = I - \text{LEFT}$$

$$= 46.3343366 \qquad \simeq 172.05826$$

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

$$= 2\left[(2+1)e^2 + (4+1)e^4\right] \qquad \text{Error} = I - \text{RIGHT}$$

$$= 590.3158369 \qquad \simeq -371.92324$$

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

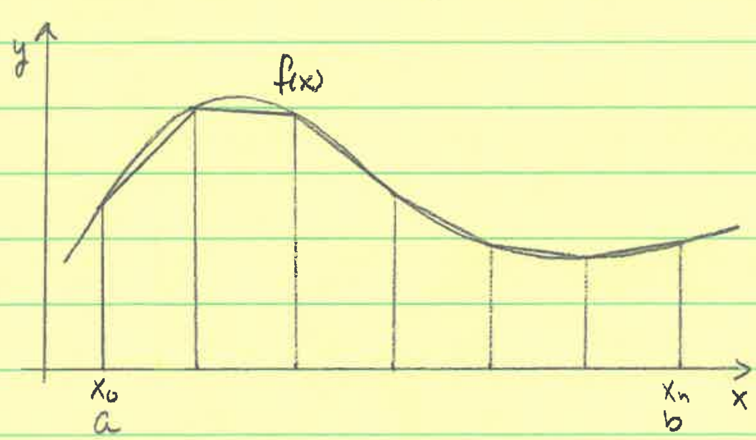
We should be able to reduce the error, however, by increasing the number of intervals.

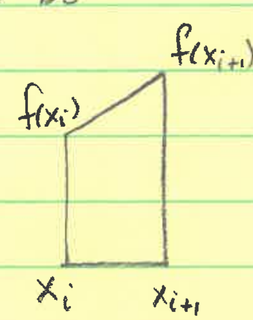
(show overhead for Left & Right Hand Sums)

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.

<u>Can we do better?</u> Yes!

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





Area = $\dfrac{f(x_i) + f(x_{i+1})}{2} \Delta x$

$\Delta x = x_{i+1} - x_i$

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

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.

	**** LEFT HAND RULE ***		*** RIGHT HAND RULE ***	
n	error	ratio	error	ratio
1	214.3926001326		-873.5704005303	
2	172.0582635390	1.25	-371.9232367924	2.35
4	109.4467204861	1.57	-162.5440296796	2.29
8	61.2518766801	1.79	-74.7434984028	2.17
16	32.3054119075	1.90	-35.6922756340	2.09
32	16.5756246874	1.95	-17.4232190833	2.05
64	8.3937341434	1.97	-8.6056877419	2.02
128	4.2233595520	1.99	-4.2763513906	2.01
256	2.1183036484	1.99	-2.1315518230	2.01
512	1.0608078393	2.00	-1.0641198964	2.00
1024	0.5308179264	2.00	-0.5316459415	2.00

This is just the average of LEFT and RIGHT:

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

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

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

(Show overhead for Midpoint & Trapezoid Rules)

Notice
1) Errors reduce by factor of 4 when # 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. (overestimates)

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.

	**** MIDPOINT RULE ****		**** TRAPEZOID RULE ***	
n	error	ratio	error	ratio
1	129.7239269454		-329.5889001989	
2	46.8351774332	2.77	-99.9324866267	3.30
4	13.0570328741	3.59	-26.5486545967	3.76
8	3.3589471348	3.89	-6.7458108613	3.94
16	0.8458374674	3.97	-1.6934318632	3.98
32	0.2118435994	3.99	-0.4237971979	4.00
64	0.0529849607	4.00	-0.1059767993	4.00
128	0.0132477447	4.00	-0.0264959193	4.00
256	0.0033120302	4.00	-0.0066240873	4.00
512	0.0008280134	4.00	-0.0016560285	4.00
1024	0.0002070037	4.00	-0.0004140076	4.00

Can we combine these rules (like we did with LEFT & 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 $\int_a^b f(x)\,dx$

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

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

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

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

$$\boxed{\text{TRAP} = \frac{b-a}{2n}\left[f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n) \right] \quad \text{where } a = x_0,\ b = x_n}$$

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.

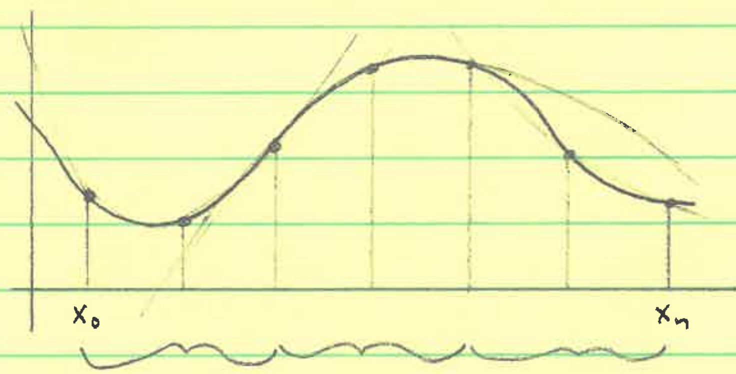
**** SIMPSON'S RULE ***

n	error	ratio
1	-23.3803487693	
2	-2.0873772534	11.20
4	-0.1448629495	14.41
8	-0.0093055305	15.57
16	-0.0005856428	15.89
32	-0.0000366664	15.97
64	-0.0000022926	15.99
128	-0.0000001433	16.00
256	-0.0000000090	16.00
512	-0.0000000006	16.00
1024	-0.0000000000	15.99

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 ...



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

$$f(x_i) = p(x_i), \quad f(x_{i+1}) = p(x_{i+1}),$$
$$f(x_{i+2}) = p(x_{i+2})$$

and note that $x_{i+1} = \dfrac{x_i + x_{i+2}}{2}$ (midpoint)

when the points are equally spaced.

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

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

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

$$\int_{x_0}^{x_n} f(x)\,dx \simeq \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2) + f(x_2) + 4f(x_3) + f(x_4)$$
$$+ f(x_4) + 4f(x_5) + f(x_6) + \cdots$$
$$\cdots + f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\Big]$$

$$= \frac{h}{3}\Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots$$
$$+ 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\Big]$$

so

$$\boxed{\begin{aligned} SIMP = \frac{b-a}{3n}\Big[&f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots \\ &\cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\Big] \\ &\text{where } a = x_0,\quad b = x_n \end{aligned}}$$

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 $[x_0, x_2]$.

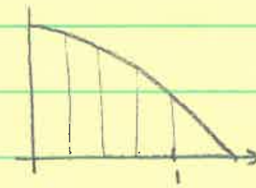
$$
\begin{aligned}
\int_{x_0}^{x_2} Ax^2 + Bx + C\,dx &= \frac{A}{3}x^3 + \frac{B}{2}x^2 + Cx\Big|_{x_0}^{x_2} \\
&= \frac{A}{3}x_2^3 + \frac{B}{2}x_2^2 + Cx_2 - \frac{A}{3}x_0^3 + \frac{B}{2}x_0^2 + Cx_0 \\
&= \frac{A}{3}(x_2^3 - x_0^3) + \frac{B}{2}(x_2^2 - x_0^2) + C(x_2 - x_0) \\
&= \frac{A}{3}(x_2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

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 $\displaystyle\int_0^1 \cos x \, dx$



Exact answer $\int_0^1 \cos x \, dx = \sin x \Big|_0^1 = \sin 1 \approx 0.84147$

Midpoint Rule with $n = 4$

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

$$= 0.84367$$

Trapezoid 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

$$\text{SIMP} = \frac{1}{12}\left[\cos(0) + 4\cos(0.25) + 2\cos(0.5) + 4\cos(0.75) + \cos(1.0)\right]$$

$$= 0.84149$$