Numerical Integration

Code used below (thanks to Al Hibbard)

Mathematica

Defining a function

To define the function $g(x) = e^{2x}\cos(x)$ in *Mathematica*, enter the following

In[1405]:=
```
g[x_] = E^(2 x) * Cos[x]
```

Notes:

- The underscore is *only* used in the definition and *only* on the left side of the equals sign.
- You must use square brackets for the argument of functions. Use round parentheses only for mathematical grouping.
- *Mathematica* is case sensitive. All built-in terms, like `Cos` and `E` begin with capital letters.
- To enter something in *Mathematica* to be calculated use the shift-enter key combination.

Derivatives

If you have defined a function like the above $f(x)$, take its derivatives using the prime notation.

In[1406]:=
```
g'[x]
```

In[1407]:=
```
g''[x]
```

In[1408]:=
```
g'''[x]
```

Summation notation

To evaluate the sum

$$\sum_{k=1}^{n} a_k$$

enter

In[1409]:=
```
Sum[a_k, {k, 1, n}]
```

For example, if $g(x)$ is the above function and $x_k = 1 + 0.02\,k$ then the Riemann sum

$$\sum_{k=1}^{100} g(1 + 0.02\,k)\,0.02$$

is

In[1410]:=
```
Sum[g[1 + 0.02 k] * 0.02, {k, 1, 100}]
```

Similar Features work in TI calculators, etc. -- e.g. sums, and lists

Review

To approximate $\int_a^b f(x)\,dx$ with n subdivisions,

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

and

$$x_k = a + k\,\Delta x$$

Numerical integration rules

- The midpoint rule for approximating $\int_a^b f(x)\,dx$ with n rectangles is

$$\int_a^b f(x)\,dx \approx f\left(\frac{x_0+x_1}{2}\right)\Delta x + f\left(\frac{x_1+x_2}{2}\right)\Delta x + \ldots + f\left(\frac{x_{n-1}+x_n}{2}\right)\Delta x\Big)$$
$$= \Delta x \sum_{k=1}^{n} f\left(a + \left(k + \frac{1}{2}\right)\Delta x\right)$$

- The trapezoid rule for approximating $\int_a^b f(x)\,dx$ with n trapezoids is

$$\int_a^b f(x)\,dx \approx \frac{\Delta x}{2}\left(f(x_0) + 2\,f(x_1) + 2\,f(x_2) + \ldots + 2\,f(x_n) + f(x_n)\right)$$
$$= \frac{\Delta x}{2}\left(f(a) + \left(2\sum_{k=1}^{n-1} f(a + k\,\Delta x)\right) + f(b)\right)$$

where $\Delta x = \frac{b-a}{n}$.

Comments/Questions to submit

Consider the integral $\int_{-1}^{1} \sqrt{1+x^2}\,dx$.

- The approximation of this using the midpoint rule with $n = 20$ is 2.295.
- The approximation of this using the trapezoid rule with $n = 20$ is 2.29677.
- The exact value (well, as computed by Mathematica), is about 2.29559.

1. Which is better, and by about how much?
2. Are you surprised? Why or why not?

Errors in numerical integration

When you approximate a quantity, typically you want to have some idea about how good your approximation is.

Error bounds

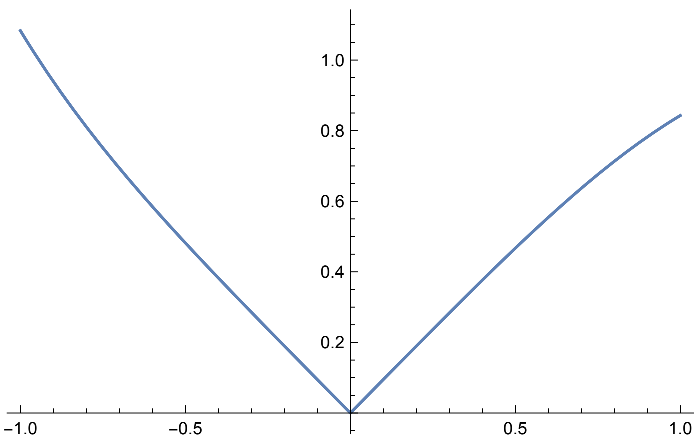
Suppose $|f''(x)| \leq K$ for $a \leq x \leq b$ where K is a constant. The error in approximating $\int_a^b f(x)\,dx$

- with the trapezoid rule using n trapezoids is error $\leq \frac{K(b-a)^3}{12n^2}$.
- with the midpoint rule using n rectangles is error $\leq \frac{K(b-a)^3}{24n^2}$.

Questions

We want to approximate $\int_{-1}^1 \sqrt{10+x^3}\,dx$. Let $f(x) = \sqrt{10+x^3}$.

3. Here's a plot of $|f''(x)|$ for $-1 \leq x \leq 1$. Looking at the graph, what is an upper bound K (a number at least as big as the maximum value) for $|f''(x)|$?



4. Determine a value of n so that the midpoint rule is guaranteed with that value of n to give an approximation with error less than 0.001, by solving the equation $\frac{K(b-a)^3}{24n^2} = 0.001$ for n. Always round up to a whole number.

- The estimate for $\int_{-1}^1 \sqrt{10+x^3}\,dx$ with the midpoint rule using that number of rectangles is 6.32344.

5. Determine a value of n so that the trapezoid rule is guaranteed with that value of n to give an approximation with error less than 0.001.

- The estimate for $\int_{-1}^1 \sqrt{10+x^3}\,dx$ with the trapezoid rule using that number of trapezoids is 6.32341.
- The true (numerical) value of the integral to that many places is 6.32342.

6. Which is better, and by about how much? Are you surprised? Why or why not?

Simpson's rule

Estimation formula

To approximate $\int_a^b f(x)\,dx$, let n be an even number and $\Delta x = \frac{b-a}{n}$, then Simpson's rule is

$$\int_a^b f(x)\,dx \approx \frac{\Delta x}{3}\left(f(x_0) + 4 f(x_1) + 2 f(x_2) + 4 f(x_3) + 2 f(x_4) + \ldots + 2 f(x_{n-2}) + 4 f(x_{n-1}) + f(x_n)\right)$$

Error bound

The error in the above approximation is

$$\text{error} \leq \frac{K(b-a)^5}{180\, n^4}$$

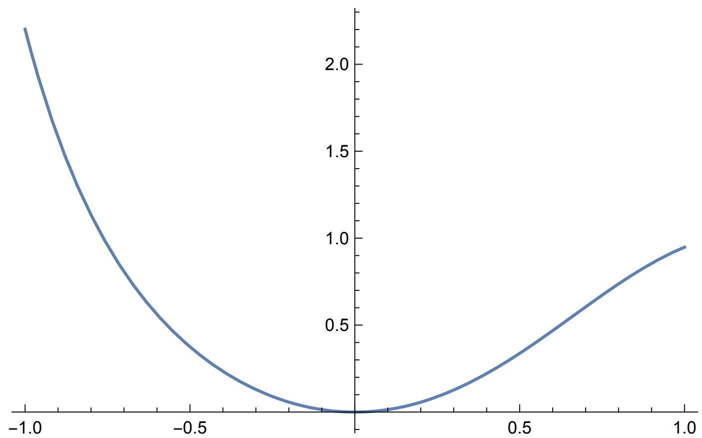
where K is a constant such that $\left| f^{(4)}(x) \right| \leq K$ for $a \leq x \leq b$.

Questions

We want to approximate $\int_{-1}^{1} \sqrt{10 + x^3}\, dx$.

8. Find an upper bound for $\left| f^{(4)}(x) \right|$ for $-1 \leq x \leq 1$ from this graph of $f^{(4)}(x)$:

Out[ ]=



9. Determine a value of n so that Simpson's rule is guaranteed with that value of n to give an approximation with error less than 0.001. **(*n* must be even for Simpson's rule.)**

10. Estimate $\int_{-1}^{1} \sqrt{10 + x^3}\, dx$ with Simpson's rule, using that value of n.

11. Compare Simpson's rule to the midpoint and trapezoidal calculations that are used in the weighted average (remember that mid and trap use n/2 rectangles).

12. How much error does each method make? Define error as estimate - true.

If you have time....

1. Verify the calculations for the rule values given in this worksheet.

2. Evaluate $\int_0^1 ln\,(x)\, dx$

3. Carry out the calculations of Stewart's problem 7.8.62, p. 575.

Let’s look at some interesting “sequences”:

In[1440]:=
```
npts = 100;
mids = Table[{n, NMidpointApprox[f[x], {x, -1, 1}, n]}, {n, 1, npts}];
mplot = ListPlot[mids]
```

In[1507]:=
```
npts = 10;
mids = Table[{n, NMidpointApprox[f[x], {x, -1, 1}, n]}, {n, 1, npts}];
traps = Table[{n, NTrapezoidApprox[f[x], {x, -1, 1}, n]}, {n, 1, npts}];
simps = (2 * mids + traps) / 3
allplots = ListPlot[{mids, traps, simps}, PlotMarkers → {{●, 10}, {▲, 10}, {■, 10}},
   PlotLegends → {"mids", "traps", "simps"}];
eplot = ListLinePlot[{{0, exact}, {npts, exact}}, PlotLegends → {"exact"}];
Show[allplots, eplot, PlotRange -> All]
```