Unit 7.1 – Numerical Integration

Numerical integration, a.k.a. Quadrature, is a sometimes-useful approach to determining the value of a definite integral, i.e.,

$$\int_a^b f(x)dx \qquad (7.1\text{-}1)$$

In a classical Calculus sense, this definite integral is defined from

$$\int_a^b f(x)dx = \lim_{\Delta x \to 0} \sum_a^b f(x)\Delta x \qquad (7.1\text{-}2)$$

The more general indefinite integral is defined a little more ambiguously, from a differential equation, i.e.,

$$F(x) + Constant = \int f(x)dx \qquad (7.1\text{-}3)$$

If

$$\frac{dF(x)}{dx} = f(x) \qquad (7.1\text{-}4)$$

Which is nice, but doesn't give us an actionable formula to find it, basically saying that you need to find the function whose derivative is…

So left to our devices, what to do? In general, as engineers we are faced with solving problems that end up being definite integrals that require a formal solution. Along the way we still frequently need the indefinite integral to set things up. We can:

1. Do Calculus like we were taught.
2. Use Wolfram
3. Use sympy

The 2 & 3 make sense in most cases. In fact, there doesn't seem to be a text problem that can't be solved this way, and to exact accuracy (sans roundoff error). However, there are problems you will likely see that require a good approximation technique. We'll talk briefly about trapezoidal rule but then move quickly into discussing the more useful Gauss quadrature, should be used for problems where the function is very expensive to calculate.

integrate from t=0 to t=2 e**(-t**2)dt

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Definite integral: More digits

$$\int_0^2 e^{-t^2}\,dt = \frac{1}{2}\sqrt{\pi}\,\mathrm{erf}(2) \approx 0.882081$$

$\mathrm{erf}(x)$ is the error function

Indefinite integral:

$$\int e^{-t^2}\,dt = \frac{1}{2}\sqrt{\pi}\,\mathrm{erf}(t) + \text{constant}$$

integrate from x=0 to x=infinity (x+3)*e**(-x)/sqrt(x) dx

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Definite integral:

$$\int_0^\infty \frac{(x+3)\,e^{-x}}{\sqrt{x}}\,dx = \frac{7\sqrt{\pi}}{2} \approx 6.20359$$

Indefinite integral:

$$\int \frac{(x+3)\,e^{-x}}{\sqrt{x}}\,dx = \frac{7}{2}\sqrt{\pi}\,\mathrm{erf}(\sqrt{x}) - e^{-x}\sqrt{x} + \text{constant}$$

integrate from x=0 to x=1 (2*x+1)/sqrt(x*(1-x))dx

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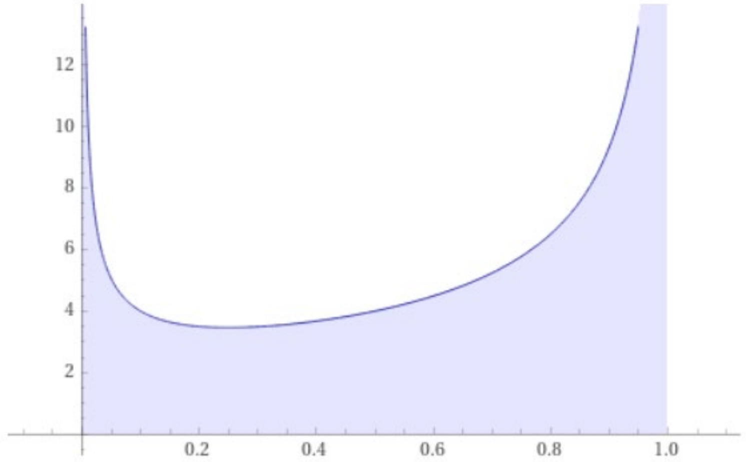
Definite integral: More digits

$$\int_0^1 \frac{2x+1}{\sqrt{x(1-x)}}\,dx = 2\pi \approx 6.2832$$

Visual representation of the integral:



So why do we want to do numerical integration if it can be done for us analytically?

Integrals

The `integrals` module in SymPy implements methods to calculate definite and indefinite integrals of expressions.

Principal method in this module is `integrate()`

- `integrate(f, x)` returns the indefinite integral $\int f\,dx$
- `integrate(f, (x, a, b))` returns the definite integral $\int_a^b f\,dx$

Examples

SymPy can integrate a vast array of functions. It can integrate polynomial functions:

Run code block in SymPy Live

```
>>> from sympy import *
>>> init_printing(use_unicode=False, wrap_line=False)
>>> x = Symbol('x')
>>> integrate(x**2 + x + 1, x)
 3    2
x    x
-- + -- + x
3    2
```

```
>>> integrate(x**2 * exp(x) * cos(x), x)
 2  x           2  x                         x           x
x *e *sin(x)   x *e *cos(x)      x          e *sin(x)   e *cos(x)
------------ + ------------ - x*e *sin(x) + --------- - ---------
     2              2                           2           2
```

even a few nonelementary integrals (in particular, some integrals involving the error function) can be evaluated:

Run code block in SymPy Live

```
>>> integrate(exp(-x**2)*erf(x), x)
  ____    2
\/ pi *erf (x)
--------------
      4
```


In sympy

N() – numeric answer

oo – infinity

Infinity() - infinity

Newton-Cotes Method

The basic idea for numerical integration can be built from the Newton-Cotes formulas in which,

$$\int_a^b f(x)dx \qquad (7.1\text{-}1)$$

Is approximated by a sum

$$I = \sum_{i=0}^{n} A_i f(x_i) \qquad (7.1\text{-}5)$$

Where the A_i are weights that are obtained based on our integration formulas. We can deal with many different formulas for this depending on the polynomial approximation we take, we could do one for the entire domain or one for each segment, like we did with splines.

The Composite Trapezoidal Rule is found by using a first order Lagrange polynomial (a straight line) fitted between nodes on the function. In other words, a piecewise straight lines, $A_0 = A_n = \frac{\Delta x}{2}$ all others $A_i = \Delta x$, assuming a constant Δx.

Piecewise quadratics lead to Simpson's 1/3 Rule, and piecewise cubics to Simpson's 3/8 Rule.

The accuracy of the approximation can be estimated and depends, as you might expect, on the function itself.

But in the end, symbolic calculus really rules the day, and it is difficult to argue that you should use a numerical technique when others are available, unless the expense of the function evaluation is so great – which does happen – or you only have the function values and not the function itself.

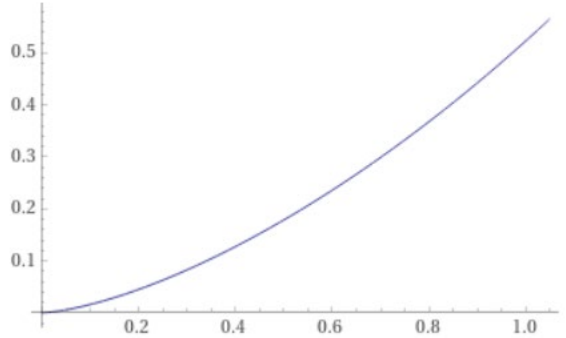
Trapezoidal Rule Example

Consider the integral: $I = \int_0^{\pi/3} \sqrt{x}\,\sin^{-1}\left(\frac{x}{2}\right) dx$

Wolfram says

$$\int_0^{\frac{\pi}{3}} \sqrt{x}\,\sin^{-1}\left(\frac{x}{2}\right) dx = \frac{2}{27}\sqrt{\frac{\pi}{3}}\left(2\left(\sqrt{36-\pi^2} - 6\,{}_2F_1\left(\frac{1}{4},\frac{1}{2};\frac{5}{4};\frac{\pi^2}{36}\right)\right) + 3\pi\sin^{-1}\left(\frac{\pi}{6}\right)\right) \approx 0.230696$$

Trapezoidal rule using 3 points says



$$\int_a^b f(x)dx = \frac{b-a}{2}\left(\frac{1}{2}f(a) + f\left(\frac{a+b}{2}\right) + f(b)\right)$$

Δx

$f(0)$

$f\left(\frac{\pi}{6}\right)$

Then:

$$\int_0^{\pi/3} \sqrt{x}\,\sin^{-1}\left(\frac{x}{2}\right) dx \approx \frac{\pi}{6}\left[\frac{1}{2}\sqrt{0}\,\sin^{-1}\left(\frac{0}{2}\right) + \sqrt{\frac{\pi}{6}}\,\sin^{-1}\left(\frac{\pi}{12}\right) + \frac{1}{2}\sqrt{\frac{\pi}{3}}\,\sin^{-1}\left(\frac{\pi}{6}\right)\right]$$
$$= 0.247994$$

Which gives 7.5% error, but hey, it's only 3 points, right?

$f\left(\frac{\pi}{3}\right)$

Unit 7.2 – Gaussian Quadrature

We again seek

$$\int_a^b f(x)dx \qquad (7.1\text{-}1)$$

approximated by a sum

$$I = \sum_{i=0}^{n} A_i f(x_i) \qquad (7.1\text{-}5)$$

The difference with Gaussian Quadrature is that we allow x_i to vary using the points that will give us the most accurate answer, the Gauss Quadrature Points.

We do this by introduce a scaling variable ξ so that (a, b) :

$$x = \frac{b+a}{2} + \frac{b-a}{2}\xi \qquad (7.2\text{-}1)$$

Turns into $(-1,1)$.

The quadrature becomes

$$\int_a^b f(x)dx = \frac{b-a}{2}\sum_{i=0}^{n} A_i f(x_i) \qquad (7.2\text{-}2)$$

Where the x_i are chosen once we decide the accuracy of the approximation from the table:

$\pm\xi_i$	A_i	$\pm\xi_i$	A_i
$n=1$		$n=4$	
0.577 350	1.000 000	0.000 000	0.568 889
$n=2$		0.538 469	0.478 629
0.000 000	0.888 889	0.906 180	0.236 927
0.774 597	0.555 556	$n=5$	
$n=3$		0.238 619	0.467 914
0.339 981	0.652 145	0.661 209	0.360 762
0.861 136	0.347 855	0.932 470	0.171 324

For comparison, let us use the same number of $f(x)$ evaluations as before, so $n = 2$.

Gauss-Legendre $\int_a^b f(x)dx = \frac{b-a}{2}\sum_{i=0}^{n} A_i f(x_i)$

$$\int_0^{\frac{\pi}{3}} \sqrt{x}\,\sin^{-1}\left(\frac{x}{2}\right)dx = \frac{2}{27}\sqrt{\frac{\pi}{3}}\left(2\left(\sqrt{36-\pi^2} - 6\,{}_2F_1\left(\frac{1}{4}, \frac{1}{2}; \frac{5}{4}; \frac{\pi^2}{36}\right)\right) + 3\pi\sin^{-1}\left(\frac{\pi}{6}\right)\right) \approx 0.230696$$

$$\int_0^{\pi/3} \sqrt{x}\,\sin^{-1}\left(\frac{x}{2}\right)dx$$

Then has $a = 0$ $\quad b = \frac{\pi}{3}$ and from 7.2-1

$$x = \frac{\pi}{6} + \frac{\pi}{6}\xi = \frac{\pi}{6}(1+\xi)$$

$\pm\xi_i$	A_i	$\pm\xi_i$	A_i
$n = 1$		$n = 4$	
0.577 350	1.000 000	0.000 000	0.568 889
$n = 2$		0.538 469	0.478 629
0.000 000	0.888 889	0.906 180	0.236 927
0.774 597	0.555 556	$n = 5$	
$n = 3$		0.238 619	0.467 914
0.339 981	0.652 145	0.661 209	0.360 762
0.861 136	0.347 855	0.932 470	0.171 324

$\xi_0 = -0.774597, \quad x_0 = 0.037567\pi, \quad A_0 = 0.555556$

$\xi_1 = 0, \quad x_1 = 0.166667\pi, \quad A_1 = 0.888889$

$\xi_2 = 0.774597, \quad x_2 = 0.295766\pi, \quad A_2 = 0.555556$

So

$$\int_0^{\pi/3} \sqrt{x}\,\sin^{-1}\left(\frac{x}{2}\right)dx \approx \frac{\pi}{6}\left[0.555556\sqrt{0.037567\pi}\,\sin^{-1}\frac{0.037567\pi}{2} + 0.888889\sqrt{0.166667\pi}\,\sin^{-1}\frac{0.166667\pi}{2} + 0.555556\sqrt{0.295766\pi}\,\sin^{-1}\frac{0.295766\pi}{2}\right]$$

$$\int_0^{\pi/3} \sqrt{x}\,\sin^{-1}\left(\frac{x}{2}\right)dx \approx 0.230589$$

Which gives 0.046% error with the same number of function evaluations

Unit 7.3 – 2D Gaussian Quadrature

To do integration in two variables the same principle applies:

$$\iint_A f(x,y)dxdy = \int_{-1}^{1}\int_{-1}^{1} f(\xi,\eta)|J(\xi,n)|\,d\xi d\eta$$

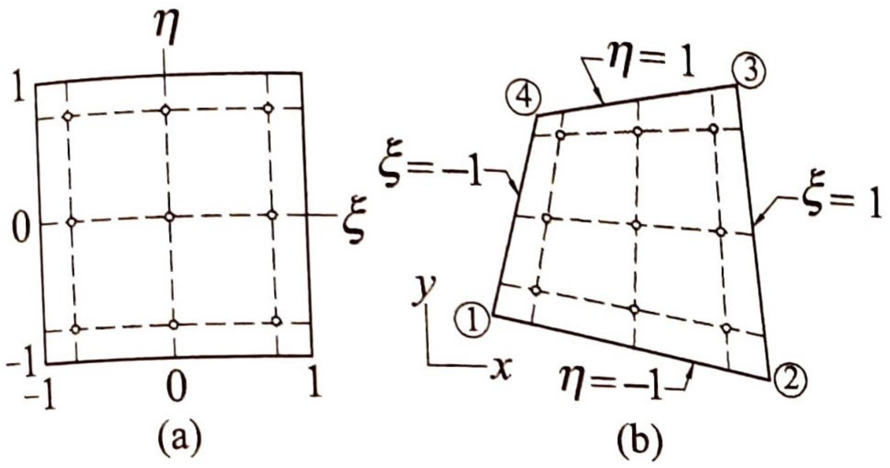
$$\approx \sum_{i=0}^{n}\sum_{j=0}^{n} A_i A_j f(x_i,y_j)\left|J(\xi_i,\eta_j)\right| \quad (7.3\text{-}1)$$

The basic idea is to introduce a mapping between (x,y) space and (ξ,η) space using the functions

$$x(\xi,\eta) = \sum_{k=1}^{4} N_k(\xi,\eta)x_k \qquad (7.3\text{-}2)$$

$$y(\xi,\eta) = \sum_{k=1}^{4} N_k(\xi,\eta)y_k \qquad (7.3\text{-}3)$$

And (x_k,y_k) are the coordinates of the corner points, and



$$N_1(\xi,\eta) = \frac{1}{4}(1-\xi)(1-\eta)$$

$$N_2(\xi,\eta) = \frac{1}{4}(1+\xi)(1-\eta)$$

$$N_3(\xi,\eta) = \frac{1}{4}(1+\xi)(1+\eta)$$

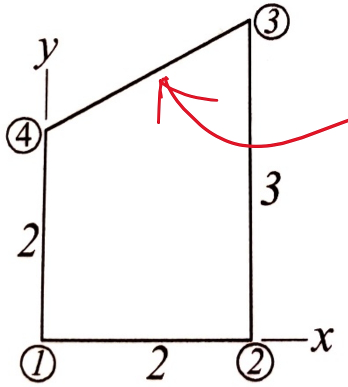
$$N_4(\xi,\eta) = \frac{1}{4}(1-\xi)(1+\eta) \qquad (7.3\text{-}4)$$

There is an alteration of the original area governed by a Jacobian matrix such that:

$$dxdy = \begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{vmatrix} d\xi d\eta \qquad (7.3\text{-}5)$$

Example 6.13

Evaluate $\iint_A (x^2 + y)dxdy$ or



$\frac{x}{2} + 2$

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$$I = \int_0^2 \int_0^{\frac{x}{2}+2} (x^2+y)\,dy\,dx$$

$$= \int_0^2 x^2 y + \frac{1}{2}y^2 \Big|_0^{\frac{x}{2}+2} dx = \int_0^2 \left[x^2\left(\frac{x}{2}+2\right) + \frac{1}{2}\left(\frac{x}{2}+2\right)^2\right] dx$$

$$= \int_0^2 \left(\frac{1}{2}x^3 + \frac{17}{8}x^2 + x + 2\right) dx$$

$$= \frac{1}{8}x^4 + \frac{17}{24}x^3 + \frac{1}{2}x^2 + 2x \Big|_0^2$$

$$= \frac{1}{\cancel{8}}(\cancel{16}^{\,2}) + \frac{17}{\cancel{24}_{\,3}}(\cancel{8}) + \frac{1}{\cancel{2}}(\cancel{4}^{\,2}) + 4 = \frac{41}{3}$$

The text example is very wrong

Now using the transformation

$$x(\xi,\eta) = \sum_{k=1}^{4} N_k(\xi,\eta)\, x_k$$

$$= \frac{1}{4}(1-\xi)\cancel{(1-\eta)}^{\,0}\,\phi + \frac{1}{\cancel{4}\,2}(1+\xi)(1-\eta)(\cancel{2}) + \frac{1}{\cancel{4}\,2}(1+\xi)(1+\eta)(\cancel{2}) + \frac{1}{4}\cancel{(1-\xi)}^{\,0}(1+\eta)\,\phi$$

$$= 1+\xi$$

$$y(\xi,\eta) = \sum_{k=1}^{4} N_k(\xi,\eta)\, y_k$$

$$= 0 + 0 + \frac{1}{4}(1+\xi)(1+\eta)(3) + \frac{1}{\cancel{4}\,2}(1-\xi)(1+\eta)(\cancel{2})$$

$$= \frac{(5+\xi)(1+\eta)}{4}$$

$$J(\xi,\eta) = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} = \begin{bmatrix} 1 & \frac{(1+\eta)}{4} \\ 0 & \frac{5+\xi}{4} \end{bmatrix} \quad \text{so} \quad |J(\xi,\eta)| = \frac{5+\xi}{4}$$

$$I = \iint_A (x^2+y)\,dx\,dy = \int_{-1}^{1}\int_{-1}^{1}\left[(1+\xi)^2 + \frac{(5+\xi)(1+\eta)}{4}\right]\frac{(5+\xi)}{4}\,d\xi\,d\eta$$

This becomes

even terms only remain

$$I=\int_{-1}^{1}\int_{-1}^{1}\left[\frac{45}{16}+\cancel{\frac{54}{16}\xi}+\frac{29}{16}\xi^2+\cancel{\frac{25}{16}\eta}+\cancel{\frac{5}{8}\xi\eta}+\cancel{\frac{1}{16}\xi^2\eta}+\cancel{\xi^3}\right]d\xi\,d\eta$$

$$=\int_{-1}^{1}\int_{-1}^{1}\left[\frac{45}{16}+\frac{29}{16}\xi^2\right]d\xi\,d\eta$$

$$=\int_{-1}^{1}\left(\frac{45}{16}\xi+\frac{29}{48}\xi^3\Big|_{-1}^{1}\right)d\eta=\int_{-1}^{1}\left(\frac{45}{8}+\frac{29}{24}\right)d\eta=\int_{-1}^{1}\frac{\overset{41}{\cancel{164}}}{\underset{6}{\cancel{24}}}d\eta$$

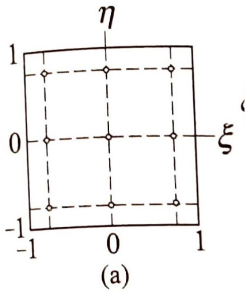
$$=\frac{41}{6}\eta\Big|_{-1}^{1}=\frac{41}{3}$$

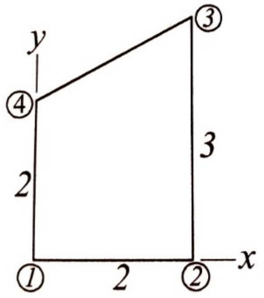
✓ so the general approach works?

What about Gauss Quadrature?

Gauss Quadrature

$$I = \sum_{i=0}^{n}\sum_{j=0}^{n} A_i A_j f(x_i, y_j)\left|J(\xi_i, \eta_j)\right|$$





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ξ	η	x_i	y_i	A_iA_j	J	$A_iA_jf(x_i,y_j)\left\|J(\xi_i,\eta_j)\right\|$
-0.774597	-0.774597	0.225403	0.238105	0.308643	1.056351	0.093942
0	-0.774597	1	0.281754	0.493828	1.25	0.791208
0.774597	-0.774597	1.774597	0.325403	0.308643	1.443649	1.548184
-0.774597	0	0.225403	1.056351	0.493828	1.056351	0.577555
0	0	1	1.25	0.790124	1.25	2.222224
0.774597	0	1.774597	1.443649	0.493828	1.443649	3.274304
-0.774597	0.774597	0.225403	1.874597	0.308643	1.056351	0.627750
0	0.774597	1	2.218246	0.493828	1.25	1.986575
0.774597	0.774597	1.774597	2.561896	0.308643	1.443649	2.544703

Sum = 13.666445
Exact = 13.666667
% Error = 0.0016%