

updated 15 February 2022

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Part 1:

Overview

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Motivation

Integrals are everywhere in physics

Some examples:

The kinetic energy- work theorem

$$\Delta K = K_f - K_i = \int_{0}^{T} \vec{F} \cdot d\vec{i}$$

Maxwell's equations, e.g., Gauss's law

$$\oint \vec{E} \cdot d\vec{A} = \frac{1}{\epsilon_0} q_{enq}$$

Fourier transforms

$$F(\omega) = \int_{\omega_i}^{\omega_f} e^{-2\pi\omega x} f(x) dx$$

Methods for evaluating integrals

Integrals can be evaluated using

- · exact integration (analytically when possible)
- simple numerical methods
- · advanced numerical methods
- We use numerical integration when
- if we cannot get an analytic answer using (many known functions, do not have an exact integral)
- the function f(x), which is to be integrated, may be a set of discrete data.

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Exact integration

Standard techniques of integration:

- substitution rule, integration by parts, using identities, ...
- · Tables of integrals
- Computer algebra systems

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Tables of integrals

- Table of Integrals, Series and Products by Gradshteyn I. S. and Ryzhik I. M. Academic Press, 1994 (many editions since 195x)
- Integral and Series, vol.1-4, by Prudnikov A P, Brychkov Yu A and Marichev A I Gordon and Breach, New York, 1986
- · Tables of Integrals and Other Mathematical Data by Herbert B. Dwight (very simple integrals, many editions)
- and many more ...



Computer algebra systems

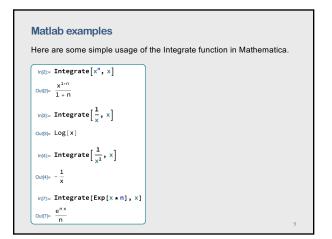
- MatLab available at ODU
- Mathematica available at ODU
- WolframAlpha https://www.wolframalpha.com/ very easy to use
- Python [Clunky]
- Maple
- Scientific Workplace
- Derive

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Matlab examples

Here are some simple usage of the int function in MATLAB.

% symbolic integrals syms x a expr = x^2*cos(x); F = int(expr) sin(x)*(x^2 - 2) + 2*x*cos(x) F = int(expr,x) expr = exp(-a*x)/A expr = exp(-a*x)/A expr = exp(-a*x)/A expr = exp(-x^2); F = int(expr) (pi^(1/2)*erf(x))/2 expr = exp(-x^2) F = int(expr,0, inf) F = pi^(1/2)/2

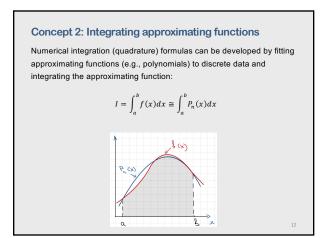




Part 2: Numerical integration: basic concepts

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Concept 1: Use the definition as a Riemann sum The definition as a Riemann sum $I = \int_{a}^{b} f(x) dx = \lim_{n \to \infty} \sum_{i=1}^{n} f(x_{i}^{*})(x_{i} - x_{i-1}) \quad a = x_{0} < x_{1} < \dots < x_{n} = b$



Integrating approximating functions (cont.)

CASE 1: The function to be integrated is known only at a finite set of discrete points.

Parameters under control - the degree of approximating polynomial

CASE 2: The function to be integrated is known.

Parameters under control:

- · The total number of discrete points
- The degree of the approximating polynomial to represent the discrete data.
- The locations of the points at which the known function is discretized

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Example: integrating direct fit polynomials

Imagine you have some discrete data in some region, and you have successfully found a polynomial to interpolate the data.

In other words, you determine the values of the coefficient, such that

$$P_n(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_k x^n = \sum_{i=1}^n a_i x$$

Then, the integral in this region is "straightforward",

$$I = \int_{a}^{b} f(x)df \approx \int_{a}^{b} P_{n}(x)dx = \sum_{i=0}^{n} \int_{a}^{b} a_{i}x^{i}dx = \sum_{i=0}^{n} a_{i}\frac{x^{i+1}}{i+1}\Big|_{a}^{b}$$

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Integrating direct fit polynomials

- This procedure only relies having determined the coefficients on the interpolating function. In other words it does not depend on whether the original data was *uniformly spaced or not*.
- Because our interpolating routines assume the data can be described by polynomials, one can imagine that this only useful for distributions whose underlying functions are non-singular.

Part 3:

Methods based on Riemann sum equal subintervals

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Riemann integral

If f(x) is a continuous function defined for $a \le x \le b$ and we divide the interval into n subintervals of equal width $\Delta x = (b - a)/n$, then the definite integral is

$$I = \int_{a}^{b} f(x) dx = \lim_{n \to \infty} \sum_{i=0}^{n} f(x_{i}^{*}) \Delta x$$

Note, for a finite n, how well the Riemann sum approximates the integral depends on, among other things, how we write the discrete sums.

The Riemann integral can be interpreted as a net area under the curve

y = f(x) from *a* to *b*.

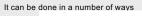
Bernhard Riemann [1826-1866]

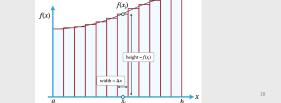
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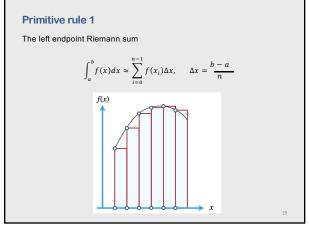
An area under the curve

Evaluating integrals exactly as an area under the curve is practically numerically impossible.

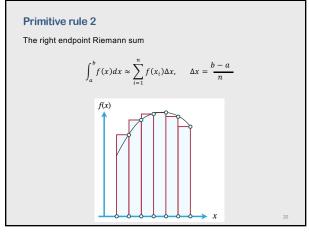
Solution: Replace this with the a "large number" of finite-sized and easyto-evaluate areas (e.g. rectangles), and have your code sum over these areas. Take the limit when these areas become increasingly small.





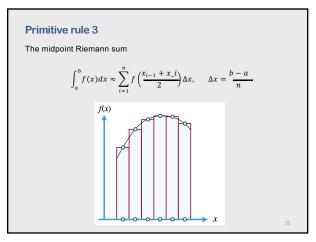




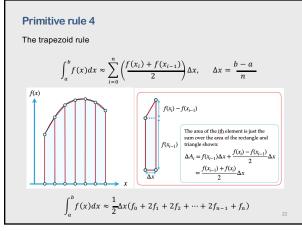




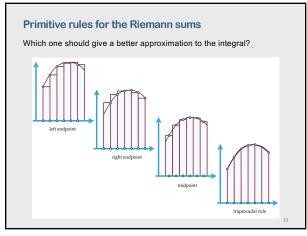




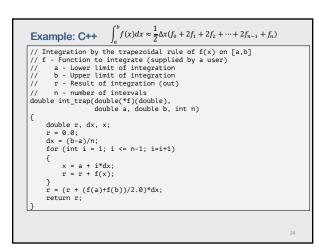










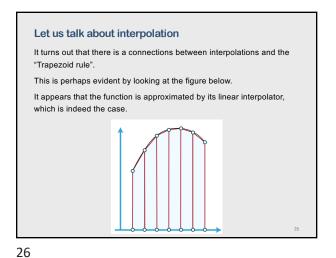




Part 3b:

Riemann sum and ... interpolation

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Let us talk about interpolation - linear interpolation

Consider the first-order interpolation for the i^{th} subinterval:

$$f(x) = f_{i-1} + \frac{f(x_i) - f(x_{i-1})}{\Lambda x} (x - x_{i-1})$$

Then, the integral for the i^{th} subinterval

$$\int_{a}^{b} f(x)dx = \int_{x_{i-1}}^{x_{i}} \left[f_{i-1} + \frac{f(x_{i}) - f(x_{i-1})}{\Delta x} (x - x_{i-1}) \right] dx = \frac{f(x_{i}) + f(x_{i-1})}{2} \Delta x$$

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which is exactly the Trapezoidal approximation!

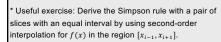
Let us talk about interpolation - quadratic interpolation

Using the three-point interpolation, e.g., 3-point Lagrange interpolation for equal subintervals, one may write Simpson's Rule for integration

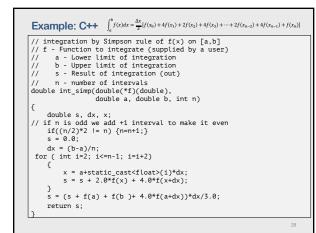
 $\int_{0}^{b} f(x)dx = \frac{\Delta x}{3} [f(x_{0}) + 4f(x_{1}) + 2f(x_{2}) + 4f(x_{3}) + \dots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_{n})]$

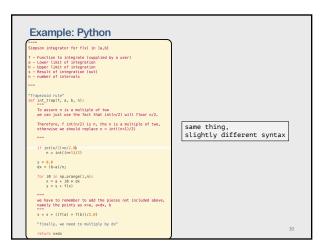
Number of n intervals should be even. If n is odd then the last interval should be treated by some other way (e.g. using the trapezoid rule).

Thomas Simpson [1710-1761]



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Part 4: **Newton-Cotes formulae**

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Newton polynomials

The direct fit polynomial procedure requires a significant amount of effort in the evaluation of the polynomial coefficients. When the function to be integrated is known at equally spaced points, the Newton difference polynomial can be fit to the discrete data with much less effort. s

$$P_{n}(x) = f_{0} + s\Delta f_{0} + \frac{s(s-1)}{2!}\Delta^{2}f_{0} + \frac{s(s-1)(s-2)}{3!}\Delta^{3}f_{0} + \cdots + \frac{s(s-1)(s-2)\dots(s-(n-1))}{n!}\Delta^{n}f_{0} + Error$$
where $s = \frac{x-x_{0}}{\Delta x} = \frac{x-x_{0}}{h}, x = x_{0} + sh$

$$Error = \left(\frac{s}{n+1}\right)h^{n+1}f^{n+1}(\xi), \quad x_{0} \le x \le x_{n}$$
Isaac Newton, 1643 - 1727

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Newton polynomials

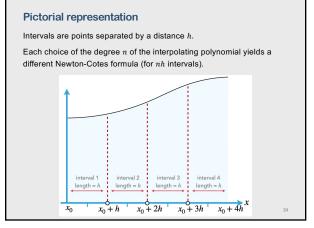
$$f = \int_{x_0}^{b} f(x) df \approx \int_{a}^{b} P_n(x) dx$$

The integral requires that the approximating polynomial be an explicit function of x, whereas the polynomial from the slide before is implicit in x. However, the integral can be transformed into an explicit function of s.

$$s = \frac{x - x_0}{h}, \qquad x = x_0 + sh, \qquad dx = hds$$
$$I = \int_a^b f(x)df \approx \int_a^b P_n(x)dx = h \int_{s(a)}^{s(b)} P_n(s)ds$$

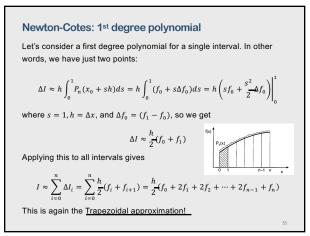
For polynomial order n we integrate from $a = x_0$ to $b = x_0 + nh$, then

 $\Delta I = h \int_0^n P_n(x_0 + sh) \, ds$

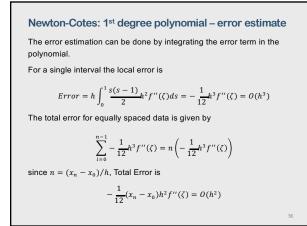












Newton-Cotes: 2nd degree polynomial

Simpson's 1/3 rule = <u>a second degree polynomial for</u> two increments (three equally spaced points). The upper limit of integration for a single interval is the s = 2

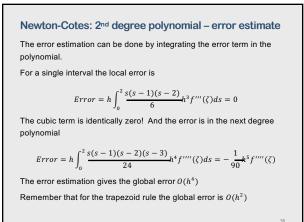
$$\Delta I \approx h \int_{0}^{2} \left(f_{0} + s\Delta f_{0} + \frac{s(s-1)}{2!} \Delta^{2} f_{0} \right) ds = \frac{h}{3} (f_{0} + 4f_{1} + f_{2})$$

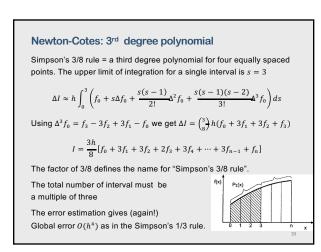
where we have used: $\Delta f_{0} = (f_{1} - f_{0}), \ \Delta^{2} f_{0} = f_{2} - 2f_{1} + f_{0}$
Applying this to all intervals we get
$$I = \frac{h}{3} [f_{0} + 4f_{1} + 2f_{2} + \dots + 2f_{n-2} + 4f_{n-1} + f_{n}]$$

This is again Simpson's rule!

The factor of 1/3 defines the name for "Simpson's 1/3 rule". The total number of interval must be even.

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Simpson's 1/3 rule vs. Simpson's 3/8 rule

Both rules have the same order for local error

$$Error_{1} = -\frac{1}{90}h^{5}f^{\prime\prime\prime\prime}(\zeta)$$
$$Error_{3} = -\frac{3}{80}h^{5}f^{\prime\prime\prime\prime}(\zeta)$$

The coefficient in the local error for 1/3 rule is even less than in the local error in 3/8 rule. Hence, Simpson's 1/3 rule should be more accurate.

Is there any value to use Simpson's 3/8 rule?

The 3/8 rule is useful when the total number of intervals is odd. Three intervals can be evaluated by the 3/8 rule and the remaining even number of intervals can be evaluated by the 1/3 rule.

But, normally, it is not worth doing it.

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Higher-order Newton-Cotes formulae

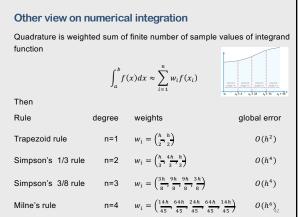
Numerical integration formulas based on equally spaced increments are called Newton- Cotes formulas. The first 10 Newton-Cotes formulas are presented in Abramowitz and Stegun (1964)*. Newton-Cotes formulas can be expressed in the general form:

$$I = \int_{-\infty}^{\infty} f(x)dx = n\beta h(\alpha_0 f_0 + \alpha_1 f_1 + \dots) + Error$$

where *n* denotes both the number of increments and the degree of the polynomial, β and α_i are coefficients

* Abramowitz and Stegun "Handbook of Mathematical Functions: with Formulas, Graphs, and Mathematical Tables" (multiple editions) see section 25 "Numerical analysis"





Integrating error

Generally as N increases, the precision of a method increases

However, as N increases, the round-off error increases Some evaluations (not exact but gives an idea)*:

Number of steps for highest accuracy:

Number of steps for highest accuracy.		
trapezoid rule	steps	error
single precision	631	3*10-6
double precision	106	10-12
Simpson's rule	steps	error
single precision	36	6*10 ⁻⁷
double precision	2154	5*10 ⁻¹⁴
* see details in R.H. Landau & M.J.Paez, An Introduction to Computational Physics		

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Integrating error (cont.)

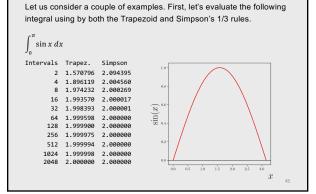
The best numerical evaluation of an integral can be obtained with a relatively small number is sub-intervals ($N \sim 1000$ or much less) (not with $N \rightarrow \infty$)

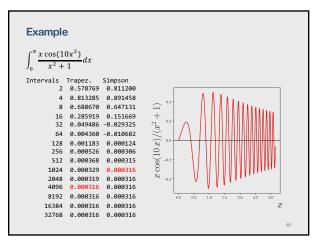
It is possible to get an error close to machine precision with Simpson's rule and with other higher-order methods (Newton-Cotes quadratures)

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Example







Key idea – use the error estimation by evaluating the integral using two different interval sizes, one with *h* and a second with a finer value of h/R where R > 1. We label these as I(h) and I(h/R).

As one can expect, the difference between these can give us an estimate of the correction needed to added to I(h/R) so as more accurately estimate the integral.



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Extrapolation and Romberg integration

The error estimate can be used both for error control and extrapolation. Consider a numerical algorithm which approximates an exact calculation with an error that depends on an increment, h

 $f_{exact} = f(h) + Ah^n + Bh^{n+m} + Ch^{n+2m} + \cdots$

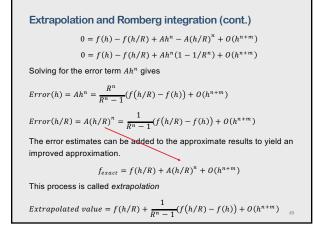
where n is the order of the leading error term and m is the increment in the order of the following error terms. Applying the algorithm at two increment sizes, $h_1 = h$ and, gives $h_2 = h/R$ gives

$$f_{exact} = f(h) + Ah^n + O(h^{n+m})$$

$$f_{exact} = f(h/R) + A(h/R)^{n} + O(h^{n+m})$$

then, the difference

 $0 = f(h) - f(h/R) + Ah^{n} - A(h/R)^{n} + O(h^{n+m})$



Extrapolation and Romberg integration (cont.)

When extrapolation is applied to numerical integration by the trapezoid rule, the result is called Romberg integration.

It can be shown that the error of the composite trapezoid rule has the functional form (the leading term is with n = 2)

 $Error = C_1h^2 + C_2h^4 + C_3h^3 + \cdots$

Let's apply the trapezoid rule for h/2 (R = 2)

$$Error(h/2) = \frac{1}{2^2 - 1} [I(h/2) - I(h)]$$

Applying the extrapolation formula gives

 $Extrapolated \ value = I(h/2) + Error(h/2) + O(h^4) =$

Extrapolated value =
$$I(h/2) + \frac{1}{2^2 - 1} [I(h/2) - I(h)] + O(h^4)$$

Thus we increased the accuracy of the trapezoid rule.

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Summary

- 1. Numerical integration is mostly based on interpolation (not on Riemann sum definition).
- The Newton-Cotes formulas, which are based on Newton forwarddifference polynomials, give simple integration formulas for equally spaced data.
- 3. Besides, Newton-Cotes formulae provide error estimates.