A Handful of Numerical Integration

Who? Minqi Pan

From? Capital Normal University

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- ... ‘cubature‘ for Numerical integration over more than one dimension

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Output an approximate solution of it!

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   - can it be written in elementary form?

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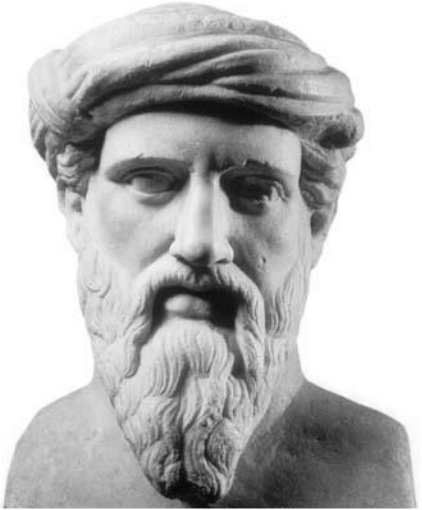
3. that's what we call symbolically

So try the other flavor

Now begins the days of Numericallarity.

It has a history!



Mathematicians of Ancient Greece, according to the Pythagorean doctrine, understood calculation of area as the process of constructing geometrically a square having the same area (squaring).

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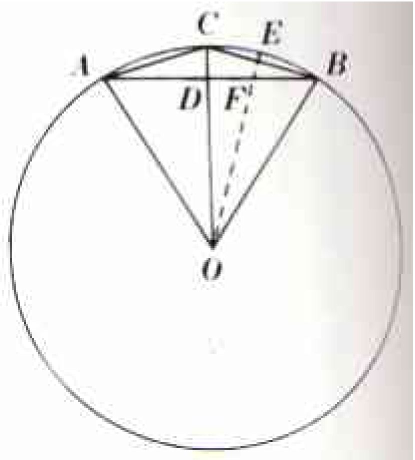
cyclotomic method by ancient Chinese Mathematician Liu Heng



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2. combine the evaluations of the integrand
3. that is, weighted sum of these values
4. get an approximation to the integral

Quadrature

Good/Bad Messures

And, **error**

1 is unavoidable

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And, **error**

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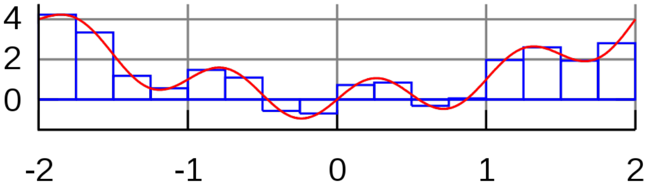
2. We want to know the number of integrand evaluations
3. result in what approximation errors?
4. small number of evaluations $\Rightarrow$ small error is good

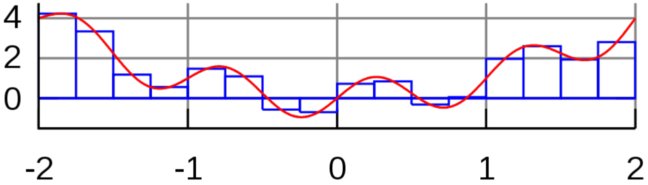
rectangular rule

$$\int_a^b f(x)\,dx \approx (b-a)\,f\left(\frac{a+b}{2}\right).$$



trapezoidal rule

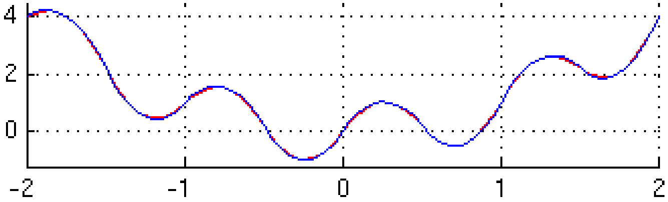
$$\int_a^b f(x)\,dx \approx (b-a)\,\frac{f(a)+f(b)}{2}.$$



Simpson's rule

$$\int_a^b f(x)\,dx \approx$$

$$\frac{b-a}{n}\left(\frac{f(a)+f(b)}{2}+\sum_{k=1}^{n-1} f\left(a+k\frac{b-a}{n}\right)\right)$$



Adaptive quadrature

If $f(x)$ does not have many derivatives at all points, or if the derivatives become large, then Gaussian quadrature is often insufficient. In this case, an algorithm similar to the following will perform better:

Extrapolation methods

The accuracy of a quadrature rule of the Newton-Cotes type is generally a function of the number of evaluation points. The result is usually more accurate as number of evaluation points increases, or, equivalently, as the width of the step size between the points decreases. It is natural to ask what the result would be if the step size were allowed to approach zero. This can be answered by extrapolating the result from two or more nonzero step sizes, using series acceleration methods such as Richardson extrapolation. The extrapolation function may be a polynomial or rational function. Extrapolation methods are described in more detail by Stoer and Bulirsch (Section 3.4) and are implemented in many of the routines in the QUADPACK library.

error estimation

Let f have a bounded first derivative over [a,b]. The mean value theorem for f, where x < b, gives

$$(x-a)f'(y_x) = f(x) - f(a)$$

for some yx in [a,x] depending on x. If we integrate in x from a to b on both sides and take the absolute values, we obtain

$$\left|\int_a^b f(x)\,dx - (b-a)f(a)\right| =$$

$$\left|\int_a^b (x-a)f'(y_x)\,dx\right|$$

Truncation error

Trunction errors in numerical integration are of two kinds:
local truncation errors Ð the error caused by one iteration, and global truncation errors Ð the cumulative error cause by many iterations.

Integrals over infinite intervals

One way to calculate an integral over infinite interval,

$$\int_{-\infty}^{+\infty} f(x)\,dx,$$

is to transform it into an integral over a finite interval by any one of several possible changes of variables, for example:

$$\int_{-\infty}^{+\infty} f(x)\,dx = \int_{-1}^{+1} f\left(\frac{t}{1-t^2}\right)\frac{1+t^2}{(1-t^2)^2}\,dt,$$

The integral over finite interval can then be evaluated by ordinary integration methods.

Multidimensional

The quadrature rules discussed so far are all designed to compute one-dimensional integrals. To compute integrals in multiple dimensions, one approach is to phrase the multiple integral as repeated one-dimensional integrals by appealing to Fubini's theorem. This approach requires the function evaluations to grow exponentially as the number of dimensions increases. Two methods are known to overcome this so-called curse of dimensionality.

Sparse grids

Sparse grids were originally developed by Smolyak for the quadrature of high dimensional functions. The method is always based on a one dimensional quadrature rule, but performs a more sophisticated combination of univariate results.

Half-infinite intervals

Monte Carlo methods and quasi-Monte Carlo methods are easy to apply to multi-dimensional integrals, and may yield greater accuracy for the same number of function evaluations than repeated integrations using one-dimensional methods.

A large class of useful Monte Carlo methods are the so-called Markov chain Monte Carlo algorithms, which include the Metropolis-Hastings algorithm and Gibbs sampling.