Numerical Integration

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Ref. ‘Methods of Numerical Integration’, Philip J. Davis and Philip Rabinowitz.

Definitions

Improper integrals → Integrals whose integrand is unbounded.

1)

- $f(x)$ is defined on $(a,b]$;
- $f(x)$ is unbounded in the neighbourhood of $x = a$.

$$\int_a^b f(x)\,dx = \lim_{r \to a^+} \int_r^b f(x)\,dx$$

2)

- $f(x)$ is defined on $[a,b] \setminus \{c\}$;
- $f(x)$ is unbounded in the vicinity of $x = c$, with $a < c < b$.

The ***Cauchy Principal Value*** of the integral is defined by the limit

$$P\int_a^b f(x)\,dx = \lim_{r \to 0^+} \left[\int_a^{c-r} f(x)\,dx + \int_{c+r}^b f(x)\,dx \right]$$

Change of variable

Sometimes it is possible to find a change of variable that eliminates the singularity.

Example 1

$g(x) \in C[0,1]$

$$I = \int_0^1 x^{-\frac{1}{n}} g(x)\,dx \qquad n \geq 2$$

The change of variable $t^n = x$ transforms the integral into

$$I = n\int_0^1 t^{n-2} g(t^n)\,dt$$

which is proper.

But (example 2)

$$I = \int_0^1 \log(x) \cdot g(x)\,dx$$

with $t = -\log x$

becomes

$$I = -\int_0^\infty t e^{-t} g(e^{-t})\,dt$$

Infinite range of integration

Elimination of the singularity

General ideas: subtract from the singular integrand $f(x)$ a function $g(x)$.

- $g(x)$ integral is known in closed form;
- $f(x)-g(x)$ is no longer singular.

This means that $g(x)$ has to mimic the behaviour of $f(x)$ closely to its singular point.

Example

$$\int_0^1 \frac{\cos x}{\sqrt{x}}dx = \int_0^1 \frac{1}{\sqrt{x}}dx + \int_0^1 \frac{\cos x - 1}{\sqrt{x}}dx = 2 + \int_0^1 \frac{\cos x - 1}{\sqrt{x}}dx.$$

But

$$\cos x - 1 \approx -\frac{x^2}{2}$$

near $x = 0$, so the last integrand in now in $C[0,1]$

Ignoring the singularity

It is also possible to avoid the integrand singularities and apply the standard quadrature rules.

We want to compute

$$\int_0^1 f(x)\,dx\,,$$

where $f(x)$ is unbounded in the neighbourhood of $x = 0$.

- Then we set $f(0) = 0$ (or any other value) and use any sequence of rules.

- Another option: use a sequence of rules that do not involve the value of $f(x)$ at $x = 0$.

Ignoring the singularity

Example 1

$$\int_0^1 \frac{dx}{\sqrt{x}} = 2$$

$32 \times S$	1.8427		G_2	1.65068
$64 \times S$	1.8887		G_3	1.75086
$128 \times S$	1.9213		G_4	1.80634
$256 \times S$	1.9444		G_{10}	1.91706
$512 \times S$	1.9606		G_{16}	1.94722
$1024 \times S$	1.9721		G_{32}	1.97321
S = Simpson			G = Gauss	

But the method of 'ignoring the singularity' may not work if the integrand is oscillatory

Example 2

$$\int_0^1 \frac{1}{x} \sin \frac{1}{x} dx = \frac{1}{2}(\pi - 2\int_0^1 \frac{\sin x}{x} dx) = .624713$$

$32 \times S$		2.3123
$64 \times S$		1.6946
$128 \times S$		-0.6083
$256 \times S$		1.2181
$512 \times S$		0.7215
$1024 \times S$		0.3178
S = Simpson		

No patterns of convergence is discernible from this computations

Ignoring the singularity

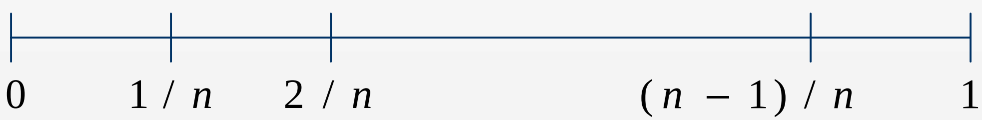
However let R designate a fixed m-point rule of approximate integration in $[0,1]$

$$R(f)=\sum_{k=1}^{m} w_k f(x_k)$$

with $\quad 0 \le x_1 < x_2 < \ldots < x_m \le 1, \quad w_k > 0, \quad \sum_{k=1}^{m} w_k = 1,$

and let R_n designate the compound rule that arises by applying R to each of the subintervals

$$[0,1/n],\ [1/n,2/n],\ldots,\ [(n-1)/n,1],$$ then



Theorem

If $f(x)$ is a monotonic increasing integrable singular function with a singularity at $x=0$, then

$$\lim_{n\to\infty} R_n(f)=\int_0^1 f(x)\,dx.$$

Proceeding to the limit

Integral to be evaluated:

$$\int_0^1 f(x)\,dx$$

- $f(x)$ is continuous in $0 < x \le 1$ (may be unbounded in $x = 0$).
- $1 > r_1 > r_2 > \ldots$ is a sequence of points that converges to 0 (e.g $r_n = 2^{-n}$).

$$\int_0^1 f(x)\,dx = \int_{r_1}^1 f(x)\,dx + \int_{r_2}^{r_1} f(x)\,dx + \int_{r_3}^{r_2} f(x)\,dx + \ldots$$

proper integrals

The evaluation is terminated when

$$\left| \int_{r_n}^{r_{n+1}} f(x)\,dx \right| \le \varepsilon$$

Truncation of the interval

$$\int_0^1 f(x)\,dx = \int_0^r f(x)\,dx + \int_r^1 f(x)\,dx$$

Then, if

$$\left| \int_0^r f(x)\,dx \right| \le \varepsilon$$

we can simply evaluate the proper integral

$$\int_r^1 f(x)\,dx$$

<u>Example</u>

$$I = \int_0^1 \frac{g(x)}{x^{\frac{1}{2}} + x^{\frac{1}{3}}}\,dx$$

with g bounded in $[0,1]$, e.g. $|g(x)| \le 1$

But in $[0,1]$

$$\left| \frac{g(x)}{x^{\frac{1}{2}} + x^{\frac{1}{3}}} \right| \le \frac{1}{2x^{\frac{1}{2}}} \quad \Longrightarrow \quad \left| \int_0^r \frac{g(x)}{x^{\frac{1}{2}} + x^{\frac{1}{3}}}\,dx \right| \le \int_0^r \frac{dx}{2x^{\frac{1}{2}}} = r^{\frac{1}{2}}$$

And, if we take $r \le 10^{-6}$, we get an accuracy of 10^{-3}

Integration Formulas of Interpolatory Type

Consider the integral

$$\int_0^1 w(x)\, f(x)\, dx$$

where $w(x)$ is a function with a singularity in the neighbourhood of $x = 0$, but such that

$$\int_0^1 w(x)\, x^k\, dx \qquad \text{exist for} \quad k = 0, 1, \ldots, n.$$

The, for a given sequence of abscissas $0 < x_0 < x_1 < \ldots x_n \le 1$, we can determine weights w_i such that

$$\int_0^1 w(x)\, p(x)\, dx = \sum_{i=0}^{n} w_i\, p(x_i)$$

whenever $p \in P_n$.

This leads to the approximate integration formula

$$\int_0^1 w(x)\, f(x)\, dx \approx \sum_{i=0}^{n} w_i\, f(x_i)$$

Integration Formulas of Interpolatory Type

Example

$$w(x) = x^{-\frac{1}{2}} \qquad x_0 = \frac{1}{3}, \quad x_1 = \frac{2}{3}, \quad x_2 = 1.$$

$$w_1 + w_2 + w_3 = \int_0^1 x^{-\frac{1}{2}} dx = 2,$$

$$\frac{w_1}{3} + \frac{2w_2}{3} + w_3 = \int_0^1 x^{-\frac{1}{2}} x dx = \frac{2}{3},$$

$$\frac{w_1}{9} + \frac{4w_2}{9} + w_3 = \int_0^1 x^{-\frac{1}{2}} x^2 dx = \frac{2}{5}.$$

This leads to the rule

$$\int_0^1 x^{-\frac{1}{2}} f(x)dx \approx \frac{14}{5} f\left(\frac{1}{3}\right) - \frac{8}{5} f\left(\frac{2}{3}\right) + \frac{4}{5} f(1).$$

Integration Formulas of Gauss Type

Singularities may be accommodated by means of Gauss-type formulas. The integral is written in the form

$$I = \int_a^b w(x) f(x)\, dx ,$$

where $w(x)$ is a fixed positive weight function. The moments

$$\int_a^b w(x) x^n \, dx \quad \text{exist for} \quad n = 0, 1, \ldots$$

but $w(x)$ may have one or more singularities in the interval $[a, b]$

The corresponding orthonormal polynomials are $p_n(x)$ and their zeros are

$$a < x_1 < x_2 < \ldots < x_n < b$$

Then $w_1, w_2, \ldots, \; w_n$ (positive constants) can be found such that

$$\int_a^b w(x) p(x)\, dx = \sum_{k=1}^{n} w_k \, p(x_k)$$

$$\int_a^b w(x) f(x)\, dx \approx \sum_{k=1}^{n} w_k \, f(x_k)$$

Integration Formulas of Gauss Type

We want to compute the integral

$$I = \int_0^1 Log(x) f(x) dx,$$

- $f(x)$ is regular in $[0,1]$

We need

$G_n(x)$ polynomials orthonormal to $Log(x)$ in $[0,1]$.

To get them, we must solve

$$I_n = \int_0^1 -Log(x)(x^n) dx.$$

- $x = e^{-y}$
- integration by parts

$$I_m = \frac{1}{m+1} \int_0^\infty e^{-(m+1)y} dy = \frac{1}{(m+1)^2}$$

Integration Formulas of Gauss Type

$$\int_0^1 -Log(x) G_i G_j \, dx = \delta_{ij}$$

• Polynomials	• Points	• Weights
$G_0 = 1,$		
$G_1 = \frac{12}{\sqrt{7}}\left(x - \frac{1}{4}\right);$	0.25	1
$G_2 = \frac{5\left(252x^2 - 180x + 17\right)}{12\sqrt{7}};$	0.602277 0.112009	0.281461 0.718539
$G_3 = \frac{7\left(258800x^3 - 310500x^2 - 92016x - 4679\right)}{9\sqrt{10849}\sqrt{647}};$	0.063891 0.368997 0.766880	0.513405 0.391980 0.094615

…

Integration Formulas of Gauss Type

- Example

$$I = \int_0^1 -\frac{Log(x)}{1+x}dx = \frac{\pi}{12} = 0.8224670.$$

n=3

$$I_{computed} = 0.8224485$$

$$I_{exact} - I_{computed} = 185 \cdot 10^{-7}$$

Numerical Evaluation of the Cauchy Principal Value

Reduction of the CPV to one-sided improper integral is possible.

$f(x)$ unbounded in $x = c$ with $a < c < b.$

Suppose that $P\int_a^b f(x)\,dx$ exists.

$$P\int_a^b f(x) = \lim_{r\to 0}\left[\int_a^{c-r} f(x)dx + \int_{c+r}^{b} f(x)dx\right]$$

Consider $c = 0$ and $b = a.$

Decompose $f(x)$ in its odd and even parts

<u>Odd</u>

$$g(x) = \frac{1}{2}[f(x) - f(-x)]$$

<u>Even</u>

$$h(x) = \frac{1}{2}[f(x) + f(-x)]$$

Numerical Evaluation of the Cauchy Principal Value

$$\int_{-a}^{-r} f(x)\,dx + \int_{r}^{a} f(x)\,dx =$$

$$\int_{-a}^{-r} g(x)\,dx + \int_{r}^{a} g(x)\,dx + \int_{-a}^{-r} h(x)\,dx + \int_{r}^{a} h(x)\,dx =$$

$$2\int_{r}^{a} h(x)\,dx.$$

Therefore

$$P\int_{-a}^{a} f(x)dx = 2\lim_{r\to 0^+}\int_{r}^{a} h(x)dx.$$

Numerical Evaluation of the Cauchy Principal Value

Example1

$$P\int_{-1}^{1}\frac{dx}{x}$$

$$h(x)=\frac{1}{2}\left(\frac{1}{x}-\frac{1}{x}\right)=0 \longrightarrow P\int_{-1}^{1}\frac{dx}{x}=0$$

Example2

$$P\int_{-1}^{1}\frac{e^{x}}{x}dx$$

$$h(x)=\frac{1}{2}\left(\frac{e^{x}}{x}+\frac{e^{-x}}{-x}\right)=\frac{1}{x}\sinh(x)$$

$$P\int_{-1}^{1}\frac{e^{x}}{x}\,dx=2\int_{0}^{1}\frac{\sinh(x)}{x}dx$$

Numerical Evaluation of the Cauchy Principal Value

The method of subtracting the singularity may also be used.

$$I(x) = P\int_a^b \frac{f(t)}{t-x}\,dt, \quad a < x < b$$

Hilbert transform of $f(x)$

$$I(x) = \int_a^b \frac{f(t)-f(x)}{t-x}\,dt + f(x)P\int_a^b \frac{dt}{t-x} =$$

$$\int_a^b \frac{f(t)-f(x)}{t-x}\,dt + f(x)\log\frac{b-x}{x-a}.$$

Consider the function

$$\phi(t,x) = \frac{f(t)-f(x)}{t-x} \qquad t \neq x,$$

$$\phi(x,x) = f\,'(x) \qquad t = x.$$

and solve

$$\int_a^b \phi(t,x)\,dt$$

∗ Interpolatory-type and Gauss-type formulas have been developed for Cauchy Principal Value integrals.

Numerical Evaluation of the Cauchy Principal Value

It may be useful to consider

$$\int_{x-h}^{x+h} \phi(t,x)\,dt = \int_{-h}^{h} \frac{f(t+x) - f(x)}{t}\,dt.$$

If $f(x)$ can be expanded in a Taylor series at $t = x$, then we have

$$\int_{x-h}^{x+h} \phi(t,x)\,dt = \int_{-h}^{h} \left(f'(x) + \frac{t\, f''(x)}{2!} + \frac{t^2\, f'''(x)}{3!} + \ldots \right) dt$$

$$= 2hf'(x) + \frac{h^3\, f'''(x)}{9} + \ldots$$

Indefinite Integration

We want to compute

$$F(x) = \int_a^x f(t)\,dt \qquad a \le x \le b$$

or the more complicated

$$F(x) = \int_a^x f(x,t)\,dt \qquad a \le x \le b$$

<u>Two choices</u>

- Regard the $F(x)$ as a definite integral over a variable range;
- Regard $F(x)$ as the solution of the differential equation

$$\frac{dF}{dx} = f(x), \qquad F(a) = 0.$$

The simplest approach:

- divide the interval of integration $a \le x \le b$ into a set of subintervals;
- apply a rule of approximate integration to each subinterval.

Simpson's rule is widely used

Indefinite Integration via Differential Equations

We can use familiar rules. Consider, for example, the classical Runge-Kutta method for the solution of

$$\frac{dy}{dx} = g(x, y) \qquad y(x_0) = y_0.$$

The relevant formulas are

$$y_{m+1} = y_m + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

$$k_1 = g(x_m, y_m), \; k_2 = g(x_m + \frac{h}{2}, y_m + \frac{hk_1}{2}),$$

$$k_3 = g(x_m + \frac{h}{2}, y_m + \frac{hk_2}{2}), \; k_2 = g(x_m + h, y_m + hk_3).$$

A general multistep method for indefinite integration would consist in computing the value of the integral at the next step, y_{n+1} in terms of the values of the integral previously computed, $y_n, y_{n-1}, \ldots,$ and in terms of the values of the integrand, $f(x_{n+1}), f(x_n), f(x_{n-1}), \ldots$

Indefinite Integration-Approximation Theory

$$F(x) = \int_a^x f(t)\,dt \qquad a \le x \le b \qquad -\infty < a < b < \infty$$

Suppose we can approximate $f(x)$ with

$$f(x) = \phi_0(x) + \phi_1(x) + \ldots + \phi_n(x) + \varepsilon(x) \qquad a \le x \le b,$$

$$|\varepsilon(x)| \le \varepsilon \qquad a \le x \le b,$$

and that

$$\psi_i(x) = \int_a^x \phi_i(t)\,dt$$

is simple to calculate.

Then

$$F(x) = \int_a^x f(t)\,dt = \psi_0(x) + \psi_1(x) + \ldots + \psi_n(x) + \eta(x),$$

with

$$|\eta(x)| = \left|\int_a^x \varepsilon(t)\,dt\right| \le (b-a)\varepsilon.$$

Indefinite Integration-Approximation Theory

Chebyshev Polynomials

$$T_n(x) = \cos(n \cdot ar\cos x) = x^n + \binom{n}{2} x^{n-2}(x^2 - 1) + \ldots$$

$$n = 0, 1, \ldots, \qquad -1 \le x \le 1$$

or

$$T_0(x) = 1, \qquad T_1(x) = x,$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \qquad n = 2, 3, \ldots,$$

If the function $f(x)$ satisfies a Lipschitz condition in $[-1,1]$, it can be expanded in an uniformely convergent series of Chebishev polynomials.

$$f(x) = \frac{1}{2}a_0 + a_1T_1(x) + a_2T_2(x) + \ldots$$

Indefinite Integration-Approximation Theory

Orthogonality

$$\int_{-1}^{1} \frac{T_m(x)T_n(x)}{\sqrt{1-x^2}}dx = \begin{cases} \pi, & m=n=0, \\ \frac{\pi}{2}, & m=n\neq 0, \\ 0, & m\neq n. \end{cases}$$

The coefficients of the series are given by

$$a_r = \frac{2}{\pi}\int_{-1}^{1} \frac{f(x)T_r(x)}{\sqrt{1-x^2}}dx = \frac{2}{\pi}\int_{0}^{\pi} f(\cos\vartheta)\cos r\vartheta d\vartheta$$

For many functions the sequence $a_0, a_1, \ldots$ decreases to zero rapidly. So

$$\int f(t)dt = \frac{a_0}{2}T_1(x) + \frac{a_1}{4}T_2(x) + \sum_{r=2} \frac{a_r}{2}\left(\frac{T_{r+1}(x)}{r+1} - \frac{T_{r-1}(x)}{r-1}\right) + cons$$