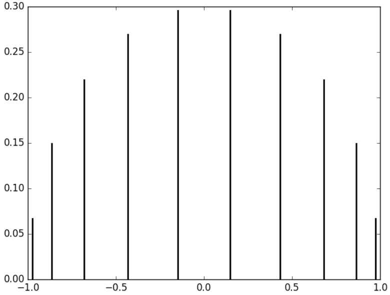
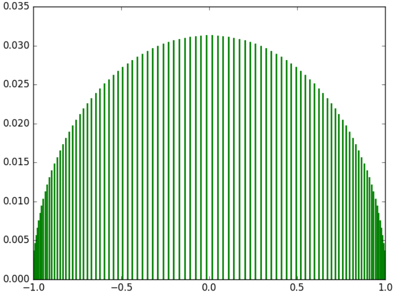
- Gaussian quadrature.
- Adaptive Integration.
- Special cases.
- Multiple integrals.

In general, in gaussian quadrature, the points are placed non-uniformly.



10 point quadrature



100 point quadrature

More points closer to the edges than in the middle.

Gaussian Quadrature

$$\int_1^2 \frac{1}{x^2} = 0.5$$

n	integral
1	0.4444444444444447
2	0.4970414201183431
3	0.4998740236835472
4	0.4999951475626201
5	0.4999998234768075
6	0.4999999938120432
7	0.4999999997886506
8	0.4999999999929189
9	0.4999999999997659
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To reach close to machine accuracy with double precision, Romberg integration needs 64 intervals, while Simpson's rule would need about 1900 intervals, and the trapezium rule would need no less than 3.8×10^6

Gaussian quadrature needs 10 points.

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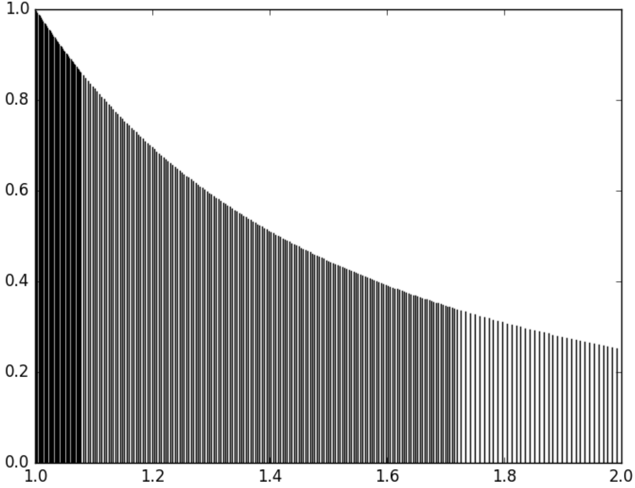
- This method – although unbiased – may often be very inefficient if the function is not equally smooth throughout the domain of integration.
- Adaptive quadrature: The domain of integration is selectively refined. This reflects the behavior of particular integrand function on a specific subinterval

Adaptive integration

Integrand is sampled densely in regions where it is difficult to integrate and sparsely in regions where it is easy.



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- Plot to see the interesting part..

Special cases

Integrals with oscillating integrands:

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Use methods or programs specially designed to calculate integrals with oscillating functions:

- Filon's method
- Clenshaw-Curtis method

Special Cases: Improper Integrals

Improper integrals integrals whose integrand is unbounded in the range of integration.

- Change of variable
- Elimination of the singularity
- Ignoring the singularity
- Truncation of the interval
- Numerical evaluation of the Cauchy Principal Value

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But one has to be careful to not trade one problem for another:

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

substituting $t = -\log(x)$,

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

Elimination of the singularity

General idea: 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.

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$$\begin{aligned}\int_0^1 \frac{\cos x}{\sqrt{x}} dx = & \int_0^1 \frac{1}{\sqrt{x}} dx + \int_0^1 \frac{\cos(x) - 1}{\sqrt{x}} dx \\ = & 2 + \int_0^1 \frac{\cos(x) - 1}{\sqrt{x}} dx\end{aligned}$$

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

But $\cos(x) - 1 \approx -\frac{x^2}{2}$ near $x = 0$ making the new integrand proper that can be integrated easily.

Ignoring the singularity

- It is also possible to avoid the integrand singularities and apply the standard quadrature formulae. If we want to compute:

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

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- Then we set $f(0) = 0$ (or any other value) and use any sequence of quadrature methods.
- Another option: use a sequence of quadrature methods that do not involve the value of $f(x)$ at $x = 0$.

Proceeding to the limit

$1 > r_1 > r_2 > \ldots$ is a sequence of points that converges to 0 (For e.g. if $r_n = 2^{-n}$, then

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

Each of the above integrals is a proper integral.
The evalulation can be terminated if

$$\left| \int_{r_n}^{r_{n+1}} f(x)dx \right| \leq \epsilon$$

Truncation of the interval

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

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For example, assume $|g(x)| < 1 \forall x \in (0, 1]$, then

$$\left| \frac{g(x)}{x^{\frac{1}{2}} + x^{\frac{1}{3}}} \right| \leq \frac{1}{2x^{\frac{1}{2}}} \implies \left| \int_0^r \frac{g(x)}{x^{\frac{1}{2}} + x^{\frac{1}{3}}} dx \right| \leq \int_0^r \frac{dx}{2x^{\frac{1}{2}}} = r^{\frac{1}{2}}$$

If we chose $r \leq 10^{-8}$. we get an accuracy of 10^{-4}.

Reduction of the CPV to one-sided improper integral is possible.
Consider $f(x)$ unbounded in $x = c$ with $a < c < b$.
Suppose that P $\int_a^b f(x)dx$ exists:

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Consider $c = 0$ and $b = -a$
Decompose $f(x)$ into its odd and even parts:

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

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

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

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

Therefore:

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

Numerical Evaluation of the Cauchy Principal Value

$$\mathsf{P}\int_{-1}^{1}\frac{1}{x}dx = 0$$

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

Numerical Evaluation of the Cauchy Principal Value

The method of subtracting the singularity may also be used.

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

$$\begin{aligned} I(x) &= \int_a^b \frac{f(t)-f(x)}{t-x}dt + f(x)\mathsf{P}\int_a^b \frac{dt}{t-x} \\ &= \int_a^b \frac{f(t)-f(x)}{t-x}dt + f(x)\log\frac{b-x}{x-a} \end{aligned}$$

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Consider the function:

$$\phi(t,x) = \frac{f(t)-f(x)}{t-x} \quad t \neq x$$
$$\phi(x,x) = f'(x) \quad t = x$$

and solve

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

It maybe useful to consider:

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

If $f(t+x)$ can be expanded in a Taylor series:

$$\int_{x-h}^{x+h} \phi(t,x)dt = \int_{-h}^{h} \left(f'(x) + \frac{tf''(x)}{2!} + \frac{t^2 f'''(x)}{3!} + \dots \right)$$
$$= 2hf'(x) + \frac{h^3 f'''(x)}{9} + \dots$$

Special cases: Indefinite integrals

$$\int_a^\infty f(x)dx \quad \int_{-\infty}^\infty f(x)dx$$

- Change of variables (common one is):

$$z = \frac{x-a}{1+x-a}$$

then

$$\int_a^\infty f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f\Big(\frac{z}{1-z} + a\Big)dz$$

- For $\int_{-\infty}^\infty$ use

$$x = \frac{z}{1-z^2} \quad \text{or} \quad x = \tan z$$

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- Replace infinite limits of integration by carefully chosen finite values. Use asymptotic behaviour to evaluate "tail" contribution! (For $a \gg 1$):

$$\begin{aligned}\int_0^\infty \frac{\sqrt{x}}{x^2+1}dx &= \int_0^a \frac{\sqrt{x}}{x^2+1}dx + \int_a^\infty \frac{\sqrt{x}}{x^2+1}dx \\ &\approx \int_0^a \frac{\sqrt{x}}{x^2+1}dx + \int_a^\infty \frac{1}{x^{3/2}}dx \\ &= \int_0^a \frac{\sqrt{x}}{x^2+1}dx + \frac{2}{\sqrt{a}}\end{aligned}$$

- Use nonlinear quadrature rules designed for infinite range intervals.

- Use automatic one-dimensional quadrature routine for each dimension, one for outer integral and another for inner integral.
- Monte-Carlo method (effective for large dimensions)

$$\int_0^1 dx_1 \int_0^1 dx_2 \cdots \int_0^1 dx_7 (x_1 + x_2 + \ldots + x_7)^2$$

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- For smooth functions all methods work well.
- For oscillating functions, functions with singularities, functions with high and narrow peaks, etc., one should use special methods and programs.
- Very good set of quadrature methods available through SciPy called QUADPACK. For your projects, use these whenever possible.