Numerical Integration

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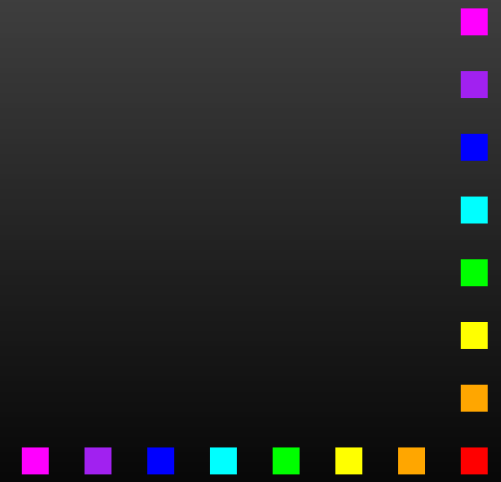


Restrictions

Integration is a wide field. We will concentrate here on Riemann integrals of the form

$$\mathrm{I}f := \int_0^1 \mathrm{d}^d x \, f(\vec{x}) \, w(\vec{x}) \, .$$

The **Weight Function** $w(\vec{x})$ is generally known analytically and is used to **absorb characteristics of the integrand** which are difficult to treat otherwise, e.g. peaks or oscillatory behaviour.

For the purposes of numerical integration, we assume that $f(\vec{x})$ **is given as a function/subroutine** that can be sampled at arbitrary points $\vec{x}_i \in [0,1]^d$.

Quadrature Formulas

Task: Find a Quadrature Formula

$$\mathrm{Q}_n f := \sum_{i=1}^{n} w_i f(\vec{x}_i)$$

with Nodes (sampling points) $\vec{x}_i$ and Weights w_i.

$\mathrm{Q}_n f$ should approximate $\mathrm{I} f$ for a large class of functions with as small an Error $\mathrm{E}_n f$ as possible:

$$\mathrm{I} f = \mathrm{Q}_n f + \mathrm{E}_n f\,, \quad \mathrm{E}_n f \text{ "small."}$$

But: For a given Q_n, it is always possible to construct an f such that $\mathrm{E}_n f$ becomes arbitrarily large!

Terminology

A **Quadrature Rule** is the vector of nodes and weights,

$$R_n = \left\{ \begin{pmatrix} \vec{x}_1 \\ w_1 \end{pmatrix}, \ldots, \begin{pmatrix} \vec{x}_n \\ w_n \end{pmatrix} \right\}$$

and of course completely specifies Q_n.

- **Open Rule** = all $\vec{x}_i$ lie strictly inside the unit hypercube.
- **Closed Rule** = some $\vec{x}_i$ lie on the boundary.
- **Positive Rule** = all w_i are positive.
  (Weights with alternating sign are generally considered inferior because numerical cancellations may occur when adding up.)

Interpolatory Formulas (1D)

Idea: **Approximate f by a polynomial $p^{(n-1)}$** and integrate the latter. Works as far as f is well approximated by polynomials.

We impose that $p^{(n-1)}$ **interpolates** f at n given points x_i:

$$p^{(n-1)}(x_i) \stackrel{!}{=} f(x_i)\,, \quad i = 1, \ldots, n\,.$$

The polynomial thus specified is unique and can explicitly be given in terms of **Lagrange Polynomials** $\ell_{n-1,i}$:

$$p^{(n-1)}(x) = \sum_{i=1}^{n} f(x_i)\ell_i^{(n-1)}(x)\,, \text{ where } \ell_i^{(n-1)}(x) = \prod_{j\neq i} \frac{x - x_j}{x_i - x_j}.$$

By construction, $\ell_i^{(n-1)}(x_j) = \delta_{ij}$.

Interpolatory Formulas (1D)

Weights:

$$\mathrm{I}\, p^{(n-1)} = \int_0^1 \mathrm{d}x\, w(x)\, p^{(n-1)}(x)$$
$$= \sum_{i=1}^{n} f(x_i) \underbrace{\int_0^1 \mathrm{d}x\, w(x)\, \ell_i^{(n-1)}(x)}_{w_i} \; .$$

From the practical point of view, the weight function $w(x)$ must be chosen such that these integrals can be computed.

The Degree of Q_n is the degree of the highest polynomial integrated exactly by Q_n.

Newton-Cotes (Rectangle) Rules (1D)

The simplest case: take equidistant x_i.
For $w(x) = 1$ the lowest-order rules are:

Open rules: $x_i = \frac{i}{n+1}$, **e.g.**

$$\mathrm{Q}_1 f = f(\tfrac{1}{2}),$$
$$\mathrm{Q}_2 f = \tfrac{1}{2}\big(f(\tfrac{1}{3}) + f(\tfrac{2}{3})\big),$$
$$\mathrm{Q}_3 f = \tfrac{1}{3}\big(2f(\tfrac{1}{4}) - f(\tfrac{1}{2}) + 2f(\tfrac{3}{4})\big).$$

Closed rules: $x_i = \frac{i-1}{n-1}$, **e.g.**

$$\mathrm{Q}_2 f = \tfrac{1}{2}\big(f(0) + f(1)\big),$$
$$\mathrm{Q}_3 f = \tfrac{1}{6}\big(f(0) + 4f(\tfrac{1}{2}) + f(1)\big),$$
$$\mathrm{Q}_4 f = \tfrac{1}{8}\big(f(0) + 3f(\tfrac{1}{3}) + 3f(\tfrac{2}{3}) + f(1)\big).$$

By construction, $\deg \mathrm{Q}_n \geqslant n - 1$, but cannot generally be expected to be larger than $n - 1$ because the x_i are prescribed and only the n w_i have been determined.

The Newton-Cotes rules by themselves are not nearly as powerful as the Gauss rules, but they have the advantage that they can be compounded easily, e.g. in Romberg Rules.

Gauss Rules (1D)

Choose the x_i such that Q_n has the highest possible degree. With $2n$ degrees of freedom (n x_i and n w_i), we ought to achieve $\deg \mathrm{Q}_n = 2n - 1$.

By Euclid's GCD algorithm we write

$$p^{(2n-1)}(x) = q^{(n)}(x)\, r^{(n-1)}(x) + s^{(n-1)}(x)\,, \qquad q^{(n)}(x) = \prod_{i=1}^{n}(x - x_i)$$

$$\mathrm{I}\, p^{(2n-1)} = \boxed{\int_0^1 \mathrm{d}x\, w(x)\, q^{(n)}(x)\, r^{(n-1)}(x)} + \int_0^1 \mathrm{d}x\, w(x)\, s^{(n-1)}(x)$$

$$= \sum_{i=1}^{n} w_i \underbrace{q^{(n)}(x_i)}_{=0} r^{(n-1)}(x_i) + \sum_{i=1}^{n} w_i\, s^{(n-1)}(x_i) + \mathrm{E}_n\, p^{(2n-1)}$$

If the boxed term were zero, the error term would vanish!

Gauss Rules (1D)

$$\int_0^1 \mathrm{d}x\, w(x)\, q^{(n)}(x)\, r^{(n-1)}(x) =$$

$$\langle q^{(n)} | r^{(n-1)} \rangle = 0 \quad \Leftrightarrow \quad q^{(n)} \perp r^{(n-1)}$$

Choose Orthogonal Polynomials for the $q^{(n)}$, then

$$r^{(n-1)} = \sum_{i=0}^{n-1} \langle q^{(i)} | r^{(n-1)} \rangle\, q^{(i)} \qquad \text{and} \quad \langle q^{(n)} | r^{(n-1)} \rangle = 0$$

$$\text{because} \quad \langle q^{(n)} | q^{(i<n)} \rangle = 0\,.$$

Since $q^{(n)}(x) = \prod_{i=1}^{n}(x - x_i)$, the x_i are just the zeros of the orthogonal polynomials $q^{(n)}$!

Gauss Rules (1D)

Gauss rules for particular weight functions have special names, hinting at the orthogonal polynomials used:

$w(x) = 1$	**Gauss-Legendre Rules**
$w(x) = 1/\sqrt{1-x^2}$	**Gauss-Chebychev Rules**
$w(x) = x^\alpha \mathrm{e}^{-x}$	**Gauss-Laguerre Rules**
$w(x) = \mathrm{e}^{-x^2}$	**Gauss-Hermite Rules**
$w(x) = (1-x)^\alpha (1+x)^\beta$	**Gauss-Jacobi Rules**

Error Estimate and Embedded Rules (1D)

So far we have **no error estimate** for our integration rule.
Idea: **Compare the results** of two rules, Q_n and Q_{n+m}.
Use **Embedded Rules** with $\{x_i\}_{i=1}^{n} \subset \{x_i\}_{i=1}^{n+m}$ for economy.
But: e.g. Gauss rules of different n have no common x_i.

Seek to add new points $x_{n+1}, \ldots, x_{n+m}$ such that Q_{n+m} is exact for polynomial of maximum degree expectable from #df, $p^{(n+2m-1)}$. This leads to

$$\int_0^1 \mathrm{d}x\, w(x)\, v^{(n)}(x)\, q^{(m)}(x)\, r^{(m-1)}(x) = 0$$

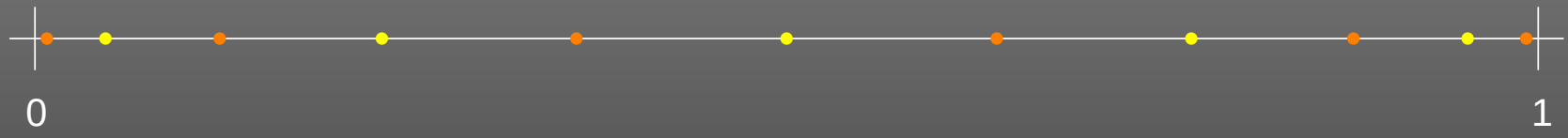
with $\quad v^{(n)}(x) = \prod_{i=1}^{n}(x - x_i)\,, \quad q^{(m)}(x) = \prod_{i=1}^{m}(x - x_{n+i})\,.$

Not all $w(x)$ have solutions since a scalar product with weight function $w(x)\, v^{(n)}(x)$ cannot in general be defined.

Embedded Rules and Null Rules

Some common **Embedded Rules** in $d = 1$ are:

- **Gauss-Kronrod Rules** add one point between every two points of a Gauss rule R_n so that $R_n \subset R_{n+n+1}$, e.g.



- **Patterson Rules** add points on top of the Gauss-Kronrod rules, e.g. there exists a set of rules
  $R_1 \subset R_3 \subset R_5 \subset R_7 \subset R_{15} \subset R_{31} \subset R_{63} \subset R_{127} \subset R_{255}$.

A **Null Rule** N_m is associated with an integration rule Q_n (usually $m < n$) and is engineered to give **zero for all functions that are integrated exactly** by Q_n.

N_m measures the "higher terms" of the integrand that are not exactly integrated by Q_n and is also used for error estimation.

Adaptive Algorithms

With an error estimate available, adaptiveness can easily be implemented:

1. Integrate the entire region: $I_{\text{tot}} \pm E_{\text{tot}}$.
2. while $E_{\text{tot}} > \max(\varepsilon_{\text{rel}} I_{\text{tot}}, \varepsilon_{\text{abs}})$
3. Find the region r with the largest error.
4. Bisect (or otherwise cut up) r.
5. Integrate each subregion of r separately.
6. $I_{\text{tot}} = \sum I_i, \;\; E_{\text{tot}} = \sqrt{\sum E_i^2}$.
7. end while

Examples: QUADPACK's QAG, CUBA's Cuhre, Suave.

Extrapolation

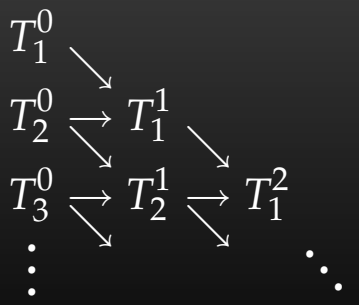
Extrapolation can be used to **accelerate convergence** if the functional behaviour of the error term is known.

Example: for the Newton-Cotes formulas the error can be shown to vary with the spacing h of the nodes as

$$\mathrm{Q}_n f - \mathrm{I} f = c_2 h^2 + c_4 h^4 + \ldots, \quad h = \frac{1}{n}\,.$$

Idea: Compute $\mathrm{Q}_n f$ for different h and extrapolate to $h = 0$.
Use **Richardson's Extrapolation** to eliminate k powers of h:

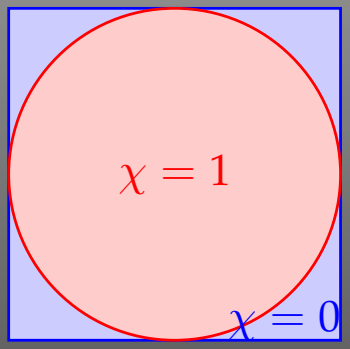
$$T_m^k := \frac{4^k T_{m+1}^{k-1} - T_m^{k-1}}{4^k - 1}\,, \quad T_m^0 := \mathrm{Q}_{2^{m-1}} f\,.$$



These are known as **Romberg Formulas.**

Curse of Dimension

Imagine computing the volume of the d-dim. sphere S_d by integrating its characteristic function $\chi = \theta(1 - \|x\|_2)$ inside the surrounding hypercube $C_d = [-1, 1]^d$.



The following table gives the ratio of the volumes:

d	2	5	10	50	100
$\frac{\text{Vol}\, S_d}{\text{Vol}\, C_d}$	.785	.164	.0025	1.5×10^{-28}	1.9×10^{-70}

This ratio can in a sense be thought of as the chance that a general-purpose integrator will find the sphere at all!

Product Formulas

Easiest method: Iterate one-dimensional rules, e.g.

$$\int_0^1 \mathrm{d}^3x\, f(\vec{x}) = \sum_{i=1}^{n_x}\sum_{j=1}^{n_y}\sum_{k=1}^{n_z} w_i^{(x)} w_j^{(y)} w_k^{(z)} f(x_i^{(x)}, x_j^{(y)}, x_k^{(z)})\,.$$

But: the number of samples increases as $N = \prod_{i=1}^{d} n_i \sim n^d$.

Consider e.g. the Newton-Cotes rules, where the error term is $\mathcal{O}(h^2) = \mathcal{O}(n^{-2})$. Convergence is thus:

$$\mathbf{Q}_n f - \mathbf{I} f = \mathcal{O}(N^{-2/d})\,.$$

Even for moderate dimensions (say $d \gtrsim 5$), this convergence rate is usually too slow to be useful.

Construction of Polynomial Rules

Select orthogonal basis of functions $\{b_1, \ldots, b_m\}$ (usually monomials) with which most f can (hopefully) be approximated sufficiently and impose that each b_i be integrated exactly by Q_n:

$$\mathrm{I}\, b_i \stackrel{!}{=} \mathrm{Q}_n b_i \quad \Leftrightarrow \quad \sum_{k=1}^{n} w_k b_i(\vec{x}_k) = \int_0^1 \mathrm{d}^d x\, w(\vec{x})\, b_i(\vec{x})\,.$$

These are m Moment Equations for $nd + n$ unknowns $\vec{x}_i$, w_i, and a formidable, in general nonlinear, system of equations.

Additional assumptions (e.g. Symmetries) are often necessary to solve this system. If a unique solution exists, Q_n is an Interpolatory Rule.

Example: the Genz–Malik rules used in CUBA's Cuhre.

Monte Carlo Methods

Idea: Interpret f as a Random Variable and estimate $\mathrm{I}f$ by the Statistical Average over independent, identically distributed samples $\vec{x}_i \in [0,1]^d$

$$\mathrm{I}f \approx \mathrm{M}_n f = \frac{1}{n}\sum_{i=1}^{n} f(\vec{x}_i) \qquad (w(\vec{x}) = 1 \text{ here}) \,.$$

The Standard Deviation is a probabilistic estimate of the integration error:

$$\sigma(\mathrm{M}_n f) = \sqrt{\mathrm{M}_n(f^2) - (\mathrm{M}_n f)^2} \,.$$

From $\sigma(\mathrm{M}_n f) = \frac{\sigma(f)}{\sqrt{n}}$, convergence is $\mathrm{M}_n f - \mathrm{I}f = \mathcal{O}(n^{-1/2})$.

Not particularly fast, but independent of the dimension d!

Variance Reduction

Variance Reduction = Methods for accelerating convergence.

In **Importance Sampling** one introduces a weight function:

$$\mathrm{I}f = \int_0^1 \mathrm{d}^d x\, w(\vec{x})\, \frac{f(\vec{x})}{w(\vec{x})}\,, \qquad w(\vec{x}) > 0\,, \quad \mathrm{I}\,w = 1\,.$$

- One must be able to sample from the distribution $w(\vec{x})$,
- f/w should be "smooth," such that $\sigma_w(f/w) < \sigma(f)$, e.g. w and f should have the same peak structure.

The ideal choice is $w(\vec{x}) = |f(\vec{x})|/\mathrm{I}f$ which has $\sigma_w(f/w) = 0$.

Example: Vegas uses a piecewise constant weight function which is successively refined, thus coming closer to $|f(\vec{x})|/\mathrm{I}f$.

Variance Reduction

Stratified Sampling works by sampling subregions. Consider:

	n samples in total region $r_a + r_b$	$n_a = n/2$ samples in r_a, $n_b = n/2$ samples in r_b
Integral	$\mathbf{I}f \approx \mathbf{M}_n f$	$\mathbf{I}f \approx \frac{1}{2}(\mathbf{M}^a_{n/2} f + \mathbf{M}^b_{n/2} f)$
Variance	$\frac{\sigma^2 f}{n}$ $= \frac{1}{2n}\left(\sigma_a^2 f + \sigma_b^2 f\right) +$ $\frac{1}{4n}\left(\mathbf{I}_a f - \mathbf{I}_b f\right)^2$	$\frac{1}{4}\left(\frac{\sigma_a^2 f}{n/2} + \frac{\sigma_b^2 f}{n/2}\right)$ $= \frac{1}{2n}\left(\sigma_a^2 f + \sigma_b^2 f\right)$

The optimal reduction of variance is for $n_a/n_b = \sigma_a f / \sigma_b f$.

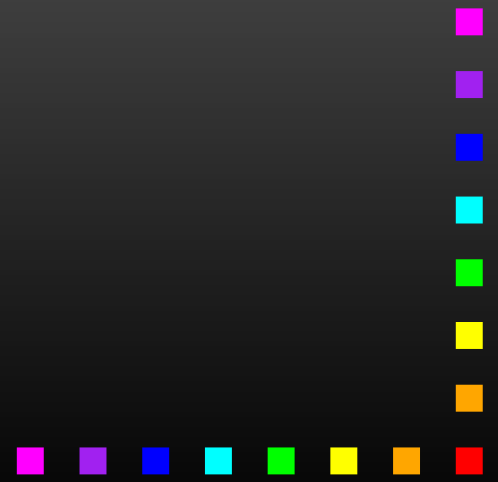
But: splitting each dimension causes a 2^d increase in regions!

Example: Miser uses Recursive Stratified Sampling.

Variance Reduction

Importance Sampling and Stratified Sampling are complementary:

- **Importance Sampling** puts most points where the magnitude of the integrand $|f|$ is largest,
- **Stratified Sampling** puts most points where the variance of f is largest.



Number-Theoretic Methods

The basis for the number-theoretical formulas is the **Koksma-Hlawka Inequality:**

The error of every $\mathrm{Q}_n f = \frac{1}{n}\sum_{i=1}^{n} f(\vec{x}_i)$ is bounded by

$$|\mathrm{Q}_n f - \mathrm{I} f| \leqslant V(f)\, D^*(\vec{x}_1, \ldots, \vec{x}_n)\,.$$

where V is the **"Variation in the sense of Hardy and Krause"** and D^* is the **Discrepancy** of the sequence $\vec{x}_1, \ldots, \vec{x}_n$,

$$D^*(\vec{x}_1, \ldots, \vec{x}_n) = \sup_{r \in [0,1]^d} \left| \frac{\nu(r)}{n} - \mathrm{Vol}\, r \right|,$$

where $\nu(r)$ counts the $\vec{x}_i$ that fall into r. For an **Equidistributed Sequence,** $\nu(r)$ should be proportional to $\mathrm{Vol}\, r$.

Low-Discrepancy Sequences and Quasi-Monte Carlo

Cannot do much about $V(f)$, but can sample with **Low-Discrepancy Sequences** a.k.a. **Quasi-Random Numbers** which have discrepancies significantly below the pseudo-random numbers used in ordinary Monte Carlo, e.g.

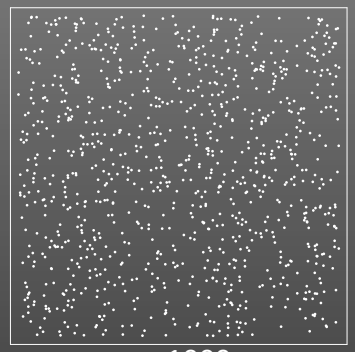
- **Halton Sequences,**
- **Sobol Sequences,**
- **Faure Sequences.**

These **Quasi-Monte Carlo Methods** typically achieve convergence rates of $\mathcal{O}(\log^{d-1} n/n)$ which are much better than the $\mathcal{O}(1/\sqrt{n})$ of ordinary Monte Carlo.

Example: CUBA's Vegas and Suave use Sobol sequences.

Comparison of Sequences

Mersenne Twister
Pseudo-Random Numbers



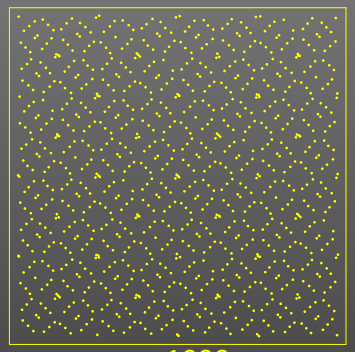
n = 1000

n = 2000

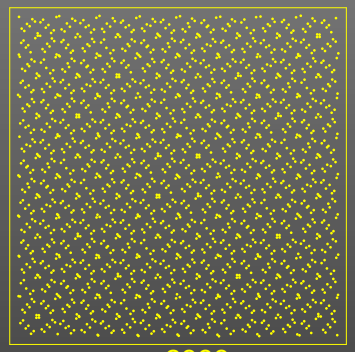
n = 3000

n = 4000

Sobol
Quasi-Random Numbers

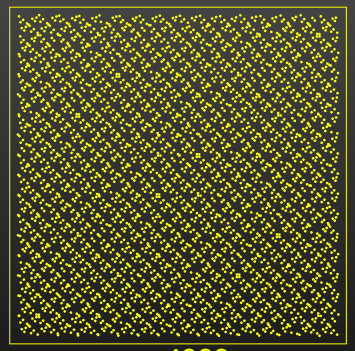


n = 1000



n = 2000

n = 3000



n = 4000

Lattice Methods

Lattice Methods require a **periodic integrand,** usually obtained by applying a **Periodizing Transformation** (e.g. $x \to 3x^2 - 2x^3$). Sampling is done on an **Integration Lattice** L spanned by a carefully selected integer vector $\vec{z}$:

$$\mathrm{Q}_n f = \frac{1}{n} \sum_{i=0}^{n-1} f\left(\left\{\tfrac{i}{n}\vec{z}\right\}\right), \quad \{x\} = \text{fractional part of } x\,.$$

Construction principle for $\vec{z}$: knock out as many low-order **"Bragg reflections"** as possible in the error term:

$$\mathrm{Q}_n f - \mathrm{I} f = \sum_{\vec{k}\in\mathbb{Z}^d} \tilde{f}(\vec{k})\,\mathrm{Q}_n \mathrm{e}^{2\pi \mathrm{i}\,\vec{k}\cdot\vec{x}} - \tilde{f}(\vec{0}) = \sum_{\vec{k}\in L^\perp,\,\vec{k}\neq\vec{0}} \tilde{f}(\vec{k})\,,$$

where $L^\perp = \{\vec{k} \in \mathbb{Z}^d : \vec{k}\cdot\vec{z} = 0 \pmod n\}$ is the **Reciprocal Lattice.** Method: extensive computer searches.

Summary

- **Univariate Integration** is pretty straightforward. **Gauss or Gauss-Kronrod/Patterson** are the rules of choice, often in an **adaptive algorithm.**

  There are, of course, many **special routines,** e.g. for oscillatory or singular integrands.

- **Multivariate Integration** is not at all straightforward. Most multivariate integrators use a more or less empirical hodge-podge of **Quadrature Rules, Monte Carlo, quasi-Monte Carlo, and Lattice Techniques,** garnished with one or more **Variance Reduction Methods.**

  There are several "good" algorithms on the market, all of which have their PROs and CONs, but there is in general no "best" algorithm.

Software

- QUADPACK, http://www.netlib.org/quadpack
  Fortran. Standard for 1D problems. Well tested. Well documented in QUADPACK book (Springer), but book out of print, README file.
- NAG (Numerical Algorithms Group), http://www.nag.co.uk
  Fortran and C. Commercial, well documented and tested.
- IMSL, http://www.imsl.com
  (Intl. Math and Statistical Libraries, now Visual Numerics)
  Fortran, C, C#, Java. Commercial, well documented and tested.
- CERNLIB, http://wwwinfo.cern.ch/asd/
  Fortran. Somewhat aged, well documented.
- CUBA, http://www.feynarts.de/cuba, hep-ph/0404043
  Fortran, C/C++, Mathematica. Quite new, well documented.

Books

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