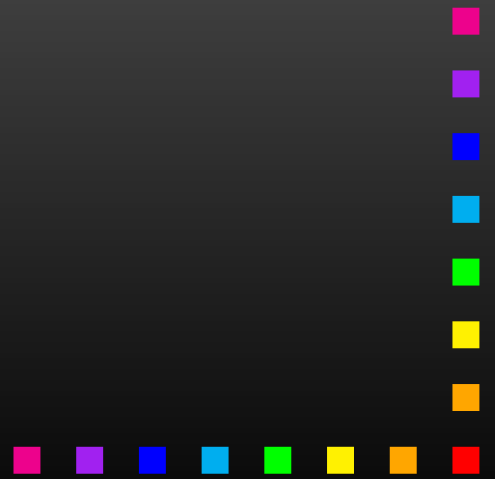
Thoughts on Numerical Integration

Thomas Hahn

Max-Planck-Institut für Physik
München



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.

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!**

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:

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

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 are not as powerful as the Gauss rules, but can be compounded easily, e.g. in Romberg Rules.

Also, extrapolation algorithms exist.

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

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

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

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

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

Gauss Rules (1D)

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

[Functional scalar product: $\langle a|b\rangle = \int_0^1 \mathrm{d}x\, w(x)\, a(x)\, b(x)\,.$]

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

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

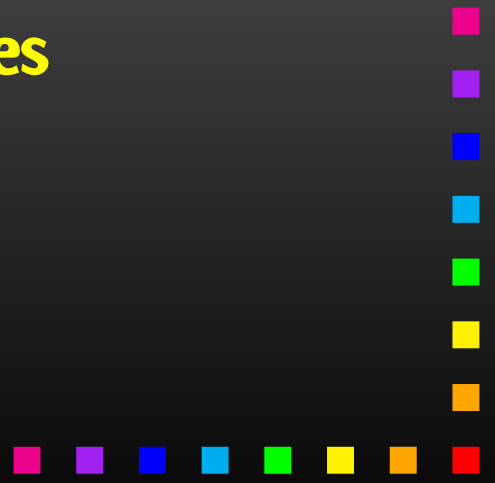
$$\text{because} \qquad \langle q^{(n)} | q^{(i<n)} \rangle = 0\,.$$

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

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

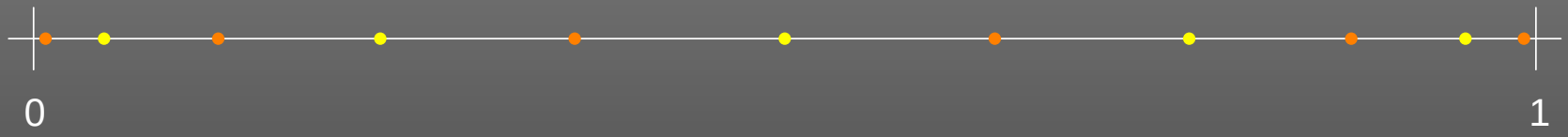
with $v^{(n)}(x) = \prod_{i=1}^{n}(x - x_i)\,, \quad q^{(m)}(x) = \prod_{i=1}^{m}(x - x_{n+i})\,.$

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:

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

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

Extrapolation

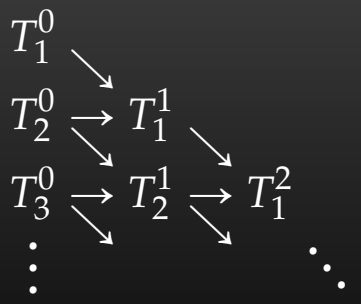
Extrapolation can be used to accelerate convergence if the functional behaviour of the error term is known.

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:

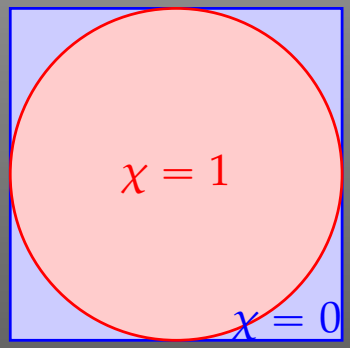
$$T_m^k := \frac{4^k T_{m+1}^{k-1} - T_m^{k-1}}{4^k - 1}, \quad T_m^0 := \mathrm{Q}_{2^{m-1}} f.$$



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	$\frac{\sigma^2 f}{n}$ $= \frac{1}{2n}(\sigma_a^2 f + \sigma_b^2 f) + \frac{1}{4n}(\mathbf{I}_a f - \mathbf{I}_b f)^2$	$\frac{1}{4}\left(\frac{\sigma_a^2 f}{n/2} + \frac{\sigma_b^2 f}{n/2}\right)$ $= \frac{1}{2n}(\sigma_a^2 f + \sigma_b^2 f)$

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

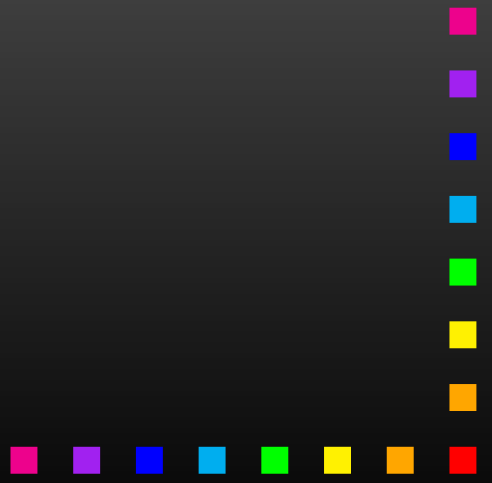
But: splitting each dimension causes a 2^d increase in regions!

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 $\mathrm{Vol}\, r$.

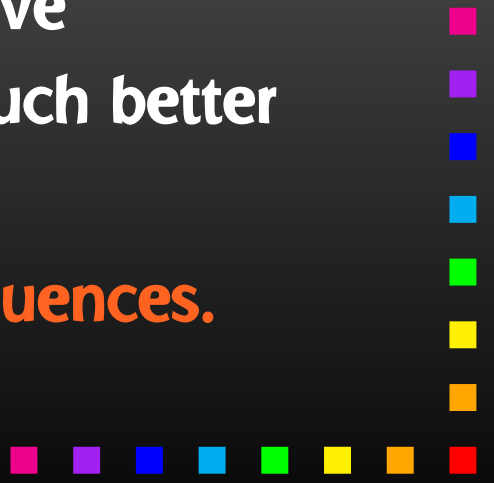
Low-Discrepancy Sequences and Quasi-Monte Carlo

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.

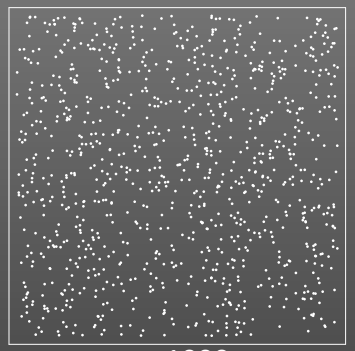
These **Quasi-Monte Carlo Methods** typically achieve convergence rates of $\mathcal{O}(\log^{d-1} n/n)$ which are much better than the $\mathcal{O}(1/\sqrt{n})$ of ordinary Monte Carlo.

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



Comparison of Sequences

Mersenne Twister
Pseudo-Random Numbers


n = 1000

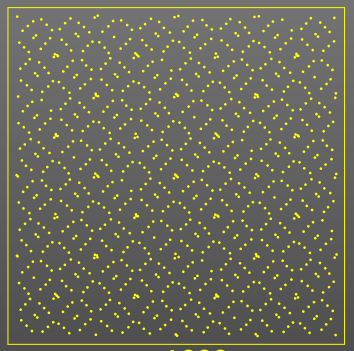

n = 2000

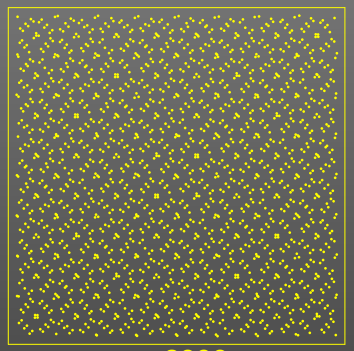

n = 3000


n = 4000

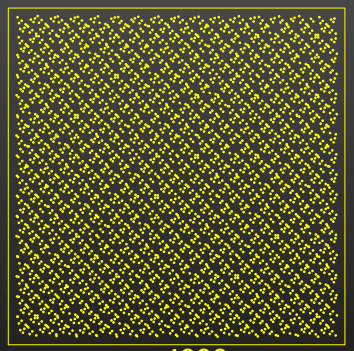
$\mathcal{O}(1/\sqrt{n})$

Sobol
Quasi-Random Numbers


n = 1000


n = 2000


n = 3000


n = 4000

$\mathcal{O}(\log^{d-1} n/n)$

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 $\vec{z}$:

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

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

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

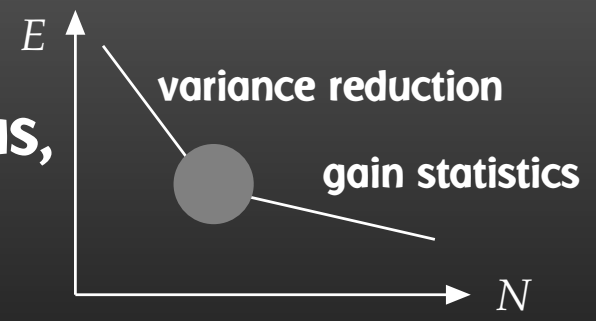
where $L^\perp = \{\vec{k} \in \mathbb{Z}^d : \vec{k}\cdot\vec{z} = 0 \pmod n\}$ is the **Reciprocal Lattice.** Method: extensive computer searches.

Machine Learning Methods

From arXiv:1707.00028:

Algorithm	# of Func. Evals	$\sigma_w / < w >$	σ_I / I (2e6 add. evts)
VEGAS	300,000	2.820	$\pm 2.0 \times 10^{-3}$
Foam	3,855,289	0.319	$\pm 2.3 \times 10^{-4}$
Generative BDT	300,000	0.082	$\pm 5.8 \times 10^{-5}$
Generative BDT (staged)	300,000	0.077	$\pm 5.4 \times 10^{-5}$
Generative DNN	294,912	0.083	$\pm 5.9 \times 10^{-5}$
Generative DNN (staged)	294,912	0.030	$\pm 2.1 \times 10^{-5}$

- gains impressive, but: only one integrand, maximally unsuited for Vegas,
- speedup only for variance reduction.



<rant> "Machine Learning" = ignorantly applying a black box (preferably named TensorFlow) to one's problem in the hope of getting a solution without really understanding how. </rant>

Routines in the CUBA Library

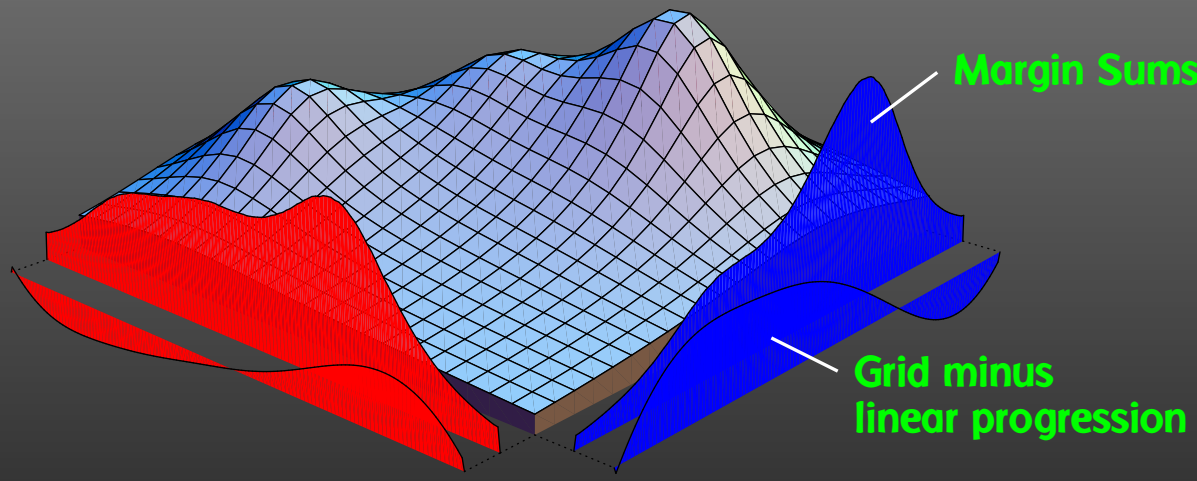
Routine	Basic method	Type	Variance reduction
Vegas	Sobol sample	Monte Carlo	importance sampling
Suave	Sobol sample	Monte Carlo	globally adaptive subdivision
Divonne	Korobov sample *or* Sobol sample *or* cubature rules	Monte Carlo Monte Carlo deterministic	stratified sampling, aided by methods from numerical optimization
Cuhre	cubature rules	deterministic	globally adaptive subdivision

- Very similar invocation (easily interchangeable)
- Fortran, C/C++, Mathematica interface provided
- Can integrate vector integrands

Vegas Overview

- Monte Carlo algorithm.
- Variance reduction: importance sampling.

▻ Iteratively build up a piecewise constant weight function on a rectangular grid.

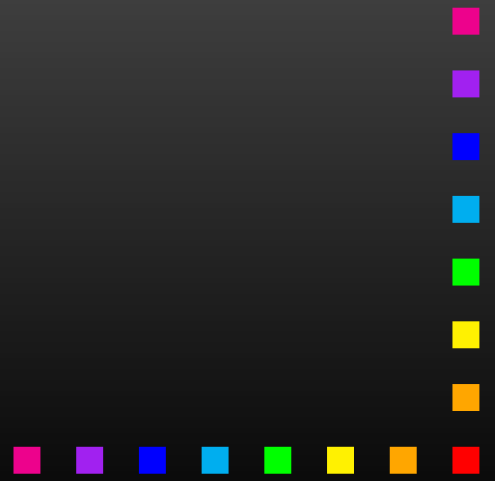


The grid shows the progression along the respective axis. Progression is slow (i.e. many points are sampled) where the grid's value is small.

▻ Each iteration consists of a sampling step followed by a refinement of the grid.

Suave Overview

- Monte Carlo algorithm.
- Variance reduction: Vegas-style importance sampling combined with globally adaptive subdivision.
  - ▻ Until the requested accuracy is reached, bisect the region with the largest error along the axis in which the fluctuations of the integrand are reduced most.
  - ▻ Prorate the number of new samples in each half for its fluctuation.



Divonne Overview

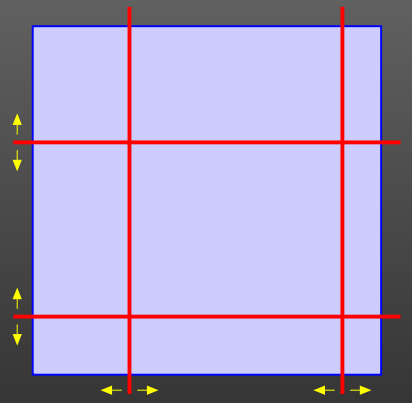
- Monte Carlo algorithm (+ cubature rules for comparison).
- Variance reduction: Stratified sampling.

▷ PHASE 1 - Partitioning

  ▷ For each subregion, 'actively' determine $\sup f$ and $\inf f$ using methods from numerical optimization.

  - Move 'dividers' around until all subregions have approximately equal spread, defined as

$$\mathrm{Spread}(r) = \frac{1}{2}\,\mathrm{Vol}(r)\Big(\sup_{\vec{x}\in r} f(\vec{x}) - \inf_{\vec{x}\in r} f(\vec{x})\Big).$$



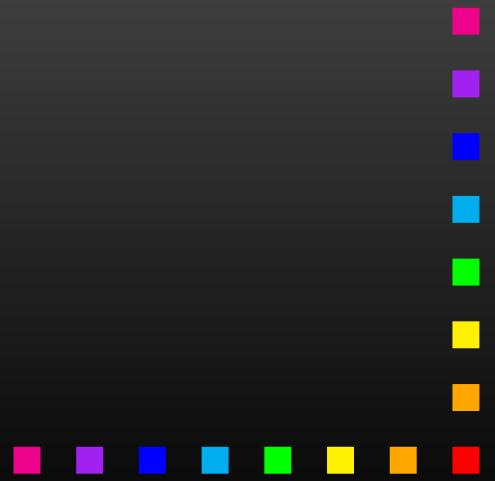
▷ PHASE 2 - Sampling: Sample the subregions independently with the same number of points each. The latter is extrapolated from the results of Phase 1.

▷ PHASE 3 - Refinement: Further subdivide or sample again if results from Phase 1 and 2 do not agree within their error.

Cuhre Overview

- Deterministic algorithm (uses cubature rules of polynomial degree).
- Variance reduction: Globally adaptive subdivision.

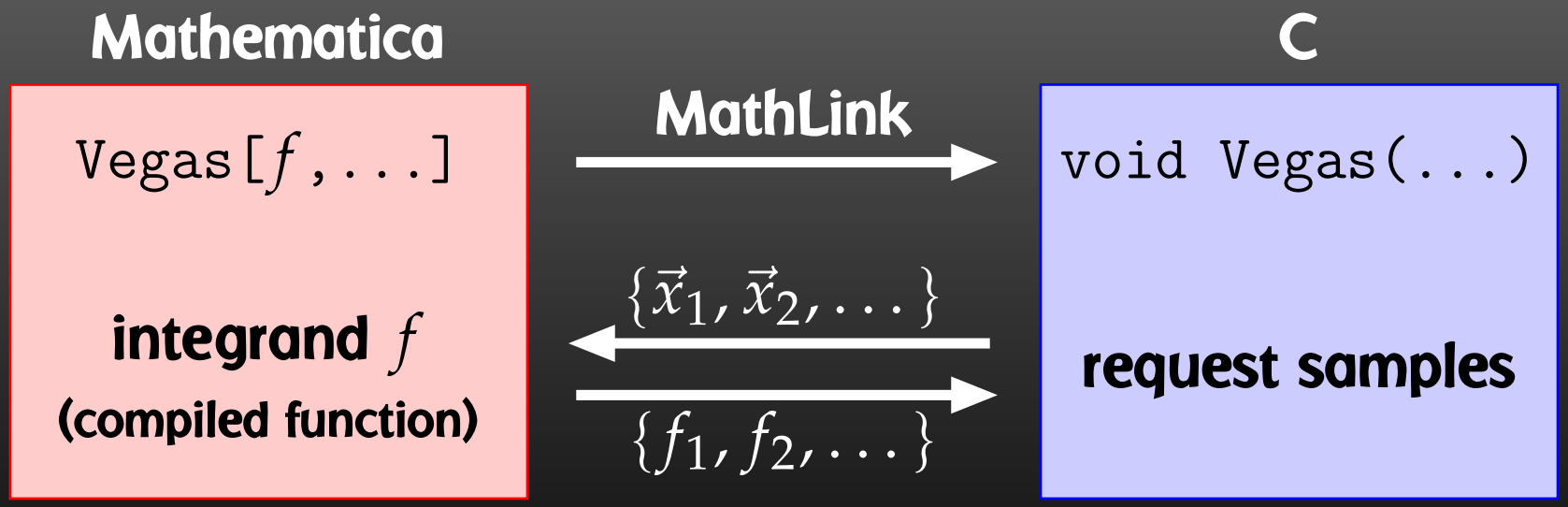
▻ Until the requested accuracy is reached, bisect the region with the largest error along the axis with the largest fourth difference.



Mathematica Interface

- **Used almost like** `NIntegrate`.
- **The integrand is evaluated completely in Mathematica. Can do things like**

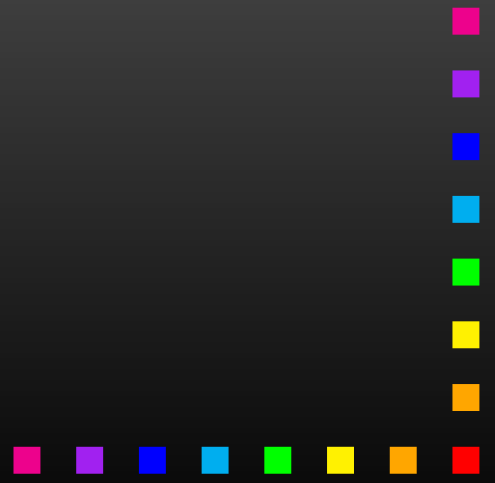
```
Cuhre[Zeta[x y], {x,2,3}, {y,4,5}]
```



Brainstorming (in lieu of a summary)

1. Physics

- How high is "high precision"?
- Need in final result? Need in subtractions?
- Perhaps try different subtraction scheme (N-jettiness?).



Brainstorming (in lieu of a summary)

2. Methodology

- Maybe only one (or few) dimensions of integration 'hard': Try to do those by 1D methods, e.g.
  - Weight function absorbs main characteristics (Gauss-XY rules).
  - Extrapolation methods.
  - Special algorithms for e.g. oscillatory integrands.
- Point out extremal points of the integrand, e.g. in Divonne.
- Combine methods, e.g. Lattice Rules "on top of" other methods.
- Explore machine-learning methods further.

Brainstorming (in lieu of a summary)

3. Technology

- Parallelize/distribute (CPU, GPU, clusters).
- Gauge precision based on (estimate of) central value of each Feynman diagram, i.e. do not waste time on unimportant parts.
- Eventually compute a grid to be used in actual calculations (Monte Carlos etc.).