Cuba

Multivariate Integration on the Hypercube

Bijan Chokoufe Nejad

Vortrag zum FOKUS-Forschungspraktikum

25 April 2013

Cuba, T. Hahn (2005), is a general purpose integrator for the hypercube $C^d = \{\boldsymbol{x} \,|\, \boldsymbol{x} \in [0,1]^d\}$,

i.e. it computes

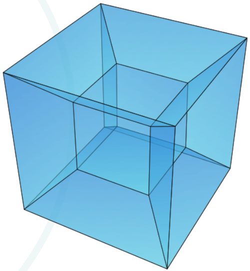
$$\mathrm{I}f = \int_0^1 \mathrm{d}^d x\, f(\boldsymbol{x}) \,.$$

Hyperrectangular regions can easily be scaled

$$\int_{a_1}^{b_1} \mathrm{d}x_1 \ldots \int_{a_n}^{b_n} \mathrm{d}x_n\, f(\boldsymbol{x})$$

$$= \prod_{i=1}^{n} \int_0^1 (b_i - a_i)\mathrm{d}y_i\, f(a_i + (b_i - a_i) y_i) \,.$$

Complicated forms can be achieved by setting $f(x) = 0$ for all x which should be excluded.



Projection of the 4-cube

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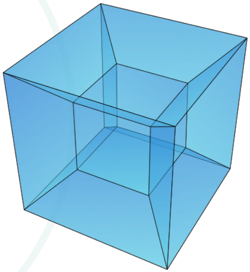

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Complicated forms can be achieved by setting $f(\boldsymbol{x}) = 0$ for all $\boldsymbol{x}$ which should be excluded.

- Completely general adaptive integration of the hypercube
- Works for easy integrands out of the box, performance can still be improved by turning the 'knobs'
- f can be given as function of x in `C/C++`, `Fortran` or `Mathematica`
- Simple interface allows usage in a broad range of Physics and other disciplines
- Parallelization via `fork` and shared memory
- Four different algorithms for cross checking

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Vegas

Standard Monte Carlo (MC) estimate of the integral and the variance

$$\bar{m}\,(f) = \frac{1}{M}\sum_{k=1}^{M} f(\boldsymbol{x}_k) \quad \text{and} \quad \bar{\sigma}(f)^2 = \frac{1}{M-1}\sum_{k=1}^{M} (f(r_k) - \bar{m}\,)^2$$

gives with the central limit theorem for large M and independent random numbers $\boldsymbol{x}_k$

$$\mathrm{I}f = \bar{m} \pm \frac{\bar{\sigma}(f)}{\sqrt{M}}\,,$$

regardless of the dimension. For variance reduction, we can use importance sampling:

$$\mathrm{I}f = \int \mathrm{d}^d x\, w(\boldsymbol{x})\,\frac{f(\boldsymbol{x})}{w(\boldsymbol{x})} = \left\langle \frac{f}{w} \right\rangle_w$$

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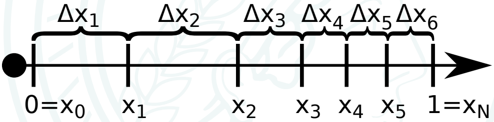
`Vegas` constructs $w(\boldsymbol{x})$ as product of piecewise-constant weight functions to minimize $\sigma(f/w)$.

The probability for a random x in any given step is equal $1/N$



The grid of Δx_i is adapted in each iteration such that the increment density is high where the margin sum of $|f|$ is large.

Main weakness of `Vegas` is sampling of peaks which are not aligned with the coordinate axes.

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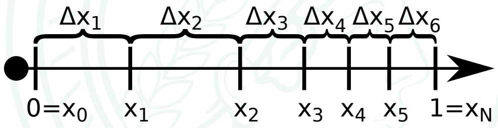

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In `Cuba`, one can choose between `MersenneTwister` and `Ranlux` by using a non-zero `seed`.

Central limit theorem only states average convergence is $1/\sqrt{N}$.

Quasi-random numbers, which are overall evenly distributed, aim to be better than average.

Number-theoretic basis is the Koksma-Hlawka inequality

$$\left| \frac{1}{N} \sum_{i=1}^{N} f(\boldsymbol{x}_i) - \int_{C^s} \mathrm{d}\boldsymbol{x}\, f(\boldsymbol{x}) \right| \leq V(f)\, D_N^*(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$$

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Variation in the sense of Hardy and Krause

$$V(f) = \sum_{k=1}^{s} \sum_{1\leq i_1<\cdots<i_k\leq s} V^{(k)}\left(f; i_1,\ldots,i_k\right) \quad \text{where}$$

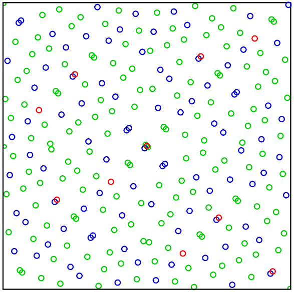
$$V^{(k)}\left(f; i_1,\ldots,i_k\right) = \int \mathrm{d}x_{i_1}\ldots\mathrm{d}x_{i_k} \left|\frac{\partial^s f}{\partial x_{i_1}\ldots\partial x_{i_k}}\right|_{x_j=1, f\neq i_1,\ldots,i_k}$$

Star-Discrepancy of a set $P = \left\{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N\right\}$

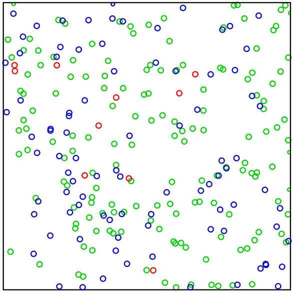
$$D_N^*(P) = \sup_{B\in J^*}\left|\frac{\#\text{ of points in } P \text{ falling into } B}{N} - \lambda(B)\right|$$

where J^* is the set of all intervals $\prod_{i=1}^{s}[0,u_i)$ and $u_i\in[0,1)$.

Sobol



Pseudo Random



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$$D_N^*(x_1, \ldots, x_N) = \mathcal{O}\left(\frac{(\log N)^s}{N}\right)$$

In general, this is not superior to PNRGs, as often claimed. Computational studies in dimension up to $s = 100$, L. Kocis *et al.* (1997), show for polynomials errors of about $\mathcal{O}\left(1/N\right)$ up to worse than $\mathcal{O}\left(1/\sqrt{N}\right)$ if the integrand has many peaks.

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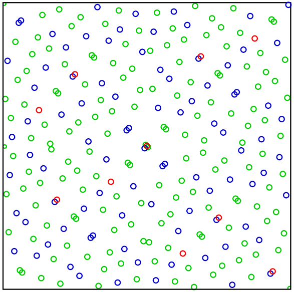

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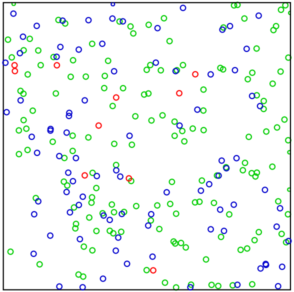

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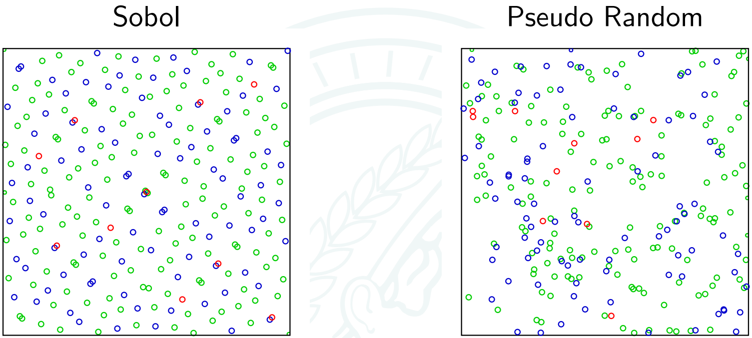

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Fairly simple: `struct state` contains all running objects

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count niter;
bool backup;
number nsamples, neval;
Cumulants cumul[NCOMP];
Grid grid[NDIM];
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Fixed size objects like this can easily be dumped to disc in C with

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fd = creat(s, 0666);
Write(fd, &state, sizeof state);
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and loaded again via

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- Integrate the whole region $\Rightarrow I_{\text{tot}} \pm E_{\text{tot}}$
- while $\Big(E_{\text{tot}} > \max\big(\epsilon_{\text{rel}} I_{\text{tot}}, \epsilon_{\text{abs}}\big)\Big)$
- Find the region r with the largest error
- Bisect r in the dimension which minimizes the fluctuations
- Sample r_L and r_R
- $I_{\text{tot}} \mathrel{+}= I_L + I_R - I_r \qquad E^2_{\text{tot}} \mathrel{+}= E^2_L + E^2_R - E^2_r$
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In Suave the points for the two new regions are distributed according to their variance which is known as stratified sampling.

Splitting up a region r in r_A and r_B leads to

$$\mathrm{I}f = \frac{1}{2}\Big(m_{N_A}(f) + m_{N_B}(f)\Big)$$

$$\sigma^2 = \frac{1}{4}\left(\frac{\sigma_A(f)^2}{N_A} + \frac{\sigma_B(f)^2}{N_B}\right)$$

Obviously, the overall variance can be reduced by making $N_{A,B}$ proportional to $\sigma_{A,B}$.

Caveat: Using too little points in each iteration, can badly underestimate the true variance in a region.

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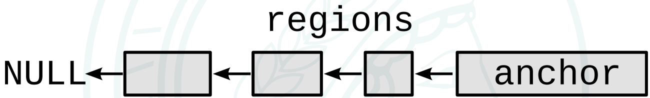

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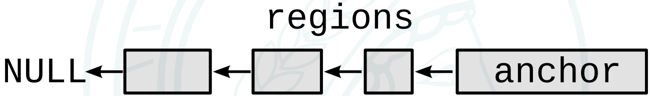

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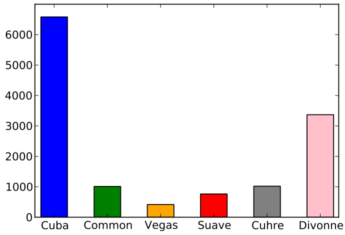
The most complex algorithm. As indicator, consider the physical lines of source code measured with `cloc-1.56`:



Divonne works in 3 phases

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- Sampling
- Refinement

and can employ 4 different samplings

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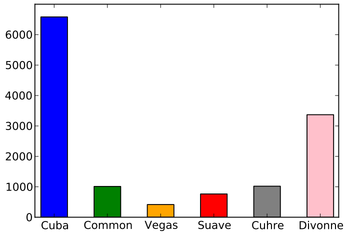

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$$s(R) = \mathrm{Vol}\,(R) \left(\max_{\boldsymbol{x}\in R} f(\boldsymbol{x}) - \min_{\boldsymbol{x}\in R} f(\boldsymbol{x}) \right)$$

Min/Max are sought with quasi-Newton method with finite difference approximations of 1st derivatives.

Partitioning: Find approximate isopleths $\tilde{f}$

$$(f^{\max} - \tilde{f})\,\mathrm{Vol}\,(R^{\max}) = (\tilde{f} - f^{\min})\,\mathrm{Vol}\left(R^{\min}\right)$$

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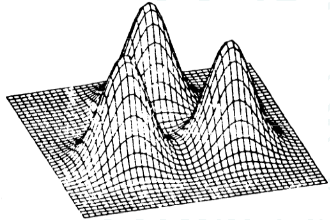
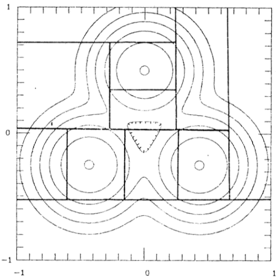
Further algorithm





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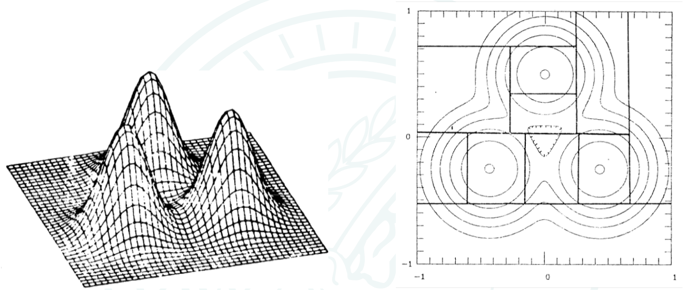
Sampling: Sample each subregion with same number of points. This number can be estimated from Phase 1.

Refinement: Subdivide or sample again if results from first phases don't agree within their error.



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Given a periodic function on C^d, the integral can be computed as

$$\int_{C^d} f(\boldsymbol{t})\mathrm{d}\boldsymbol{t} \approx \frac{1}{M}\sum_{n=1}^{M} f\left(\frac{n}{M}\,\boldsymbol{g}\right) \quad \text{with} \quad M \geq 2\,.$$

$\boldsymbol{g} \in \mathbb{Z}^d$ is a suitably chosen lattice point.

Due to periodicity, $\frac{n}{M}\,\boldsymbol{g} = \{\frac{n}{M}\,\boldsymbol{g}\}$ (the fractional part).

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$$f(\boldsymbol{t}) = \sum_{\boldsymbol{h}\in\mathbb{Z}^s} c_{\boldsymbol{h}} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{h}\boldsymbol{t}} \qquad c_{\boldsymbol{h}} = \int_{C^s} \mathrm{d}\boldsymbol{t}\, f(\boldsymbol{t}) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{h}\boldsymbol{t}}$$

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\frac{1}{M}\sum_{n=1}^{M} f\left(\frac{n}{M}\boldsymbol{g}\right) - \int_{C^s} \mathrm{d}\boldsymbol{t}\, f(\boldsymbol{t}) &= \frac{1}{M}\sum_{n}\sum_{\boldsymbol{h}} c_{\boldsymbol{h}} \mathrm{e}^{2\pi\mathrm{i}\frac{n}{M}\boldsymbol{h}\boldsymbol{g}} - c_0 \\
&= \frac{1}{M}\sum_{\boldsymbol{h}\neq\boldsymbol{0}} c_{\boldsymbol{h}} \underbrace{\sum_{n=1}^{M} \mathrm{e}^{2\pi\mathrm{i}\frac{n}{m}\boldsymbol{h}\boldsymbol{g}}}_{\begin{cases} = 0 & \text{for } \boldsymbol{h}\boldsymbol{g} \neq 0 \mod m \\ = M & \text{for } \boldsymbol{h}\boldsymbol{g} = 0 \mod m \end{cases}} \\
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&= \frac{1}{M}\sum_{\boldsymbol{h}\neq\boldsymbol{0}} c_{\boldsymbol{h}} \underbrace{\sum_{n=1}^{M} \mathrm{e}^{2\pi\mathrm{i}\frac{n}{m}\boldsymbol{h}\boldsymbol{g}}}_{\begin{cases} = 0 & \text{for } \boldsymbol{h}\boldsymbol{g} \neq 0 \mod m \\ = M & \text{for } \boldsymbol{h}\boldsymbol{g} = 0 \mod m \end{cases}} \\
&= \sum_{\substack{\boldsymbol{h}\neq\boldsymbol{0} \\ \boldsymbol{h}\boldsymbol{g}=0 \mod m}} c_{\boldsymbol{h}} \,,
\end{aligned}$$

which is the reason why Korobov benefits from smooth functions which can be described with a finite number of coefficients.

Consider

$$f(\boldsymbol{t}) = \sum_{\boldsymbol{h}\in\mathbb{Z}^s} c_{\boldsymbol{h}} \mathrm{e}^{2\pi\mathrm{i}\boldsymbol{h}\boldsymbol{t}} \qquad c_{\boldsymbol{h}} = \int_{C^s} \mathrm{d}\boldsymbol{t}\, f(\boldsymbol{t}) \mathrm{e}^{-2\pi\mathrm{i}\boldsymbol{h}\boldsymbol{t}}$$

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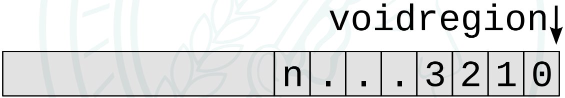
`struct` for the cumulants and fixed size regions joined together in one big chunk



Have to continue in the right phase and remember the used random numbers.

Cuhre

Cuhre is a deterministic algorithm of Berntsen, Espelid, Genz & Malik.

Integrates via one of five fully symmetric integration rules R of polynomial degree $d = 2m+1$, integrating exactly all monomials $x_1^{k_1} \ldots x_n^{k_n}$ with $\sum k_i \le d$,

$$\mathrm{I}f = \int \mathrm{d}\boldsymbol{x}\, f(\boldsymbol{x}) \simeq R[f] = \sum_{j=1}^{L} w_j f(\boldsymbol{x}_j)$$

Additionally, there are four null rules N_i of degree $2m-1$, $2m-1$, $2m-3$ and $2m-5$ for error estimation with

$$N_i[f] = \sum_{j=1}^{L} w_j^{(i)} f(\boldsymbol{x}_j), \quad i \in \{1,2,3,4\}$$

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- Same variance reduction scheme as in Suave: Globally adaptive subdivision.
- In low to moderate dimensions very accurate predictions are possible, particularly if the integrand is well approximated by polynomials.
- Memory layout is similar to Suave but with fixed size linked pools of regions

Further contributions

- Detected numerical instability in grid adaption in Vegas
- Found two Segmentation Faults in Divonne
- Fixed a bug in Cuhre which lead to negative χ^2 and wrong weights
- Updated demo files and Mathematica interfaces
- Reconsidering the `LAST` option which can lead to bad convergence and wrong results

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