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Fachrichtung Physik, Hauptseminar Monte-Carlo-Methoden

Monte-Carlo integration: Adaptive methods (VEGAS)

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Characteristics of this algorithm:

a) A reliable error estimate for the integral is readily computed.

b) The integrand need not be continuous for the algorithm to function and, in particular, step functions pose no problem. Thus integration over hypervolumes of irregular shape is straightforward.

c) The convergence rate is independent of the dimension of the integral.

d) The algorithm is adaptive. It automatically concentrates evaluations of the integrand in those regions where the integrand is largest in magnitude.

G. Peter Lepage, 1977: „A New Algorithm for Adaptive Multidimensional Integration “

Stratified sampling

$$\int_0^1 dx f(x) = \int_0^a dx f(x) + \int_a^1 dx f(x), \quad 0 < a < 1$$

- dividing the full integration space into k subspaces
- performing a Monte Carlo integration in each subspace

$$E = \sum_{j=1}^{k} \frac{\mathrm{vol}(M_j)}{N_j} \sum_{n=1}^{N_j} f(x_{jn})$$

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Importance sampling

$$\int dx\ f(x) = \int \frac{f(x)}{p(x)} p(x) dx = \int \frac{f(x)}{p(x)} dP(x)$$

$$\int dx\ p(x) = 1$$

$$p(x) = \frac{\partial^d}{\partial x_1 ... \partial x_d} P(x)$$

$$E = \frac{1}{N} \sum_{n=1}^{N} \frac{f(x_n)}{p(x_n)}$$

- change of integration variables with adequate probability density function p(x)
- random numbers distributed according to P(x)

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VEGAS algorithm

$$p_{optimal}(x) = \frac{|f(x)|}{\int dx |f(x)|}$$

Exploratory phase:

- subdivide integration space into rectangular grid
- perform integration in each subspace
- adjust grid according to dominant contributions
- integrate again, approximate $p_{optimal}$

Evalutation phase:

- integrate with high precision and optimized frozen grid

VEGAS algorithm

estimate E_j of iteration j

$$E_j = \frac{1}{N_j} \sum_{n=1}^{N_j} \frac{f(x_n)}{p(x_n)}$$

estimate for the variance S^2_j

$$S_j^2 = \frac{1}{N_j} \sum_{n=1}^{N_j} \left(\frac{f(x_n)}{p(x_n)} \right)^2 - E_j^2$$

cummulative estimate (m iterations in evaluation phase), weighted by number of calls N_j and variances S^2_j

$$E = \left(\sum_{j=1}^{m} \frac{N_j}{S_j^2} \right)^{-1} \left(\sum_{j=1}^{m} \frac{N_j E_j}{S_j^2} \right)$$

VEGAS algorithm

cummulative estimate

$$E = \left(\sum_{j=1}^{m} \frac{N_j}{S_j^2} \right)^{-1} \left(\sum_{j=1}^{m} \frac{N_j E_j}{S_j^2} \right)$$

χ^2 per degree of freedom

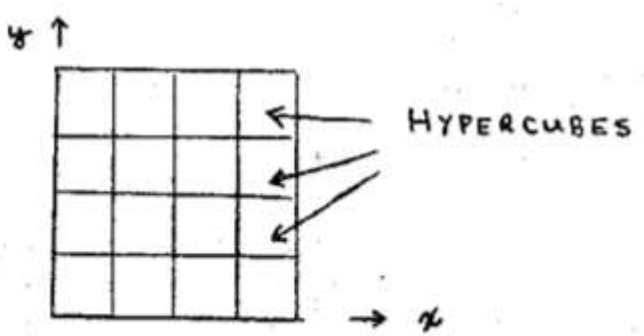
$$\chi^2/\mathrm{dof} = \frac{1}{m-1} \sum_{j=1}^{m} \frac{(E_j - E)^2}{S_j^2}$$

VEGAS algorithm (d-dimensional)

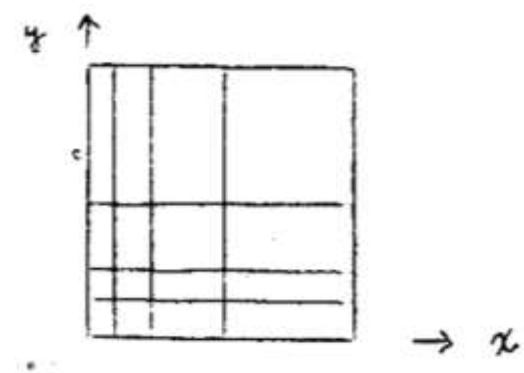
separable probability density function in d dimensions

$$p(u_1, \ldots, u_d) \quad = \quad p_1(u_1) \cdot p_2(u_2) \cdot \ldots \cdot p_d(u_d)$$

rectangular grid of hypercubes



peak at the origin, adjusted grid



Adaptive Monte Carlo methods: VEGAS

- effective, especially in high dimensions or with nonanalytic integrands
- algorithm’s requirements grow only linearly with dimension
- should be effective even in very high dimension ($n < 20$)
- quality of the estimate depends on grid adjustment

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Sources

Stefan Weinzierl, 2000:
Introduction to Monte Carlo methods
- Common introduction and overview

G. Peter Lepage, 1977:
A New Algorithm for Adaptive Multidimensional Integration
- Original paper with description and performance analysis

G. Peter Lepage, 1980:
Vegas: An Adaptive Multidimensional Integration Program
- Short theoretical considerations and description of the Fortran program VEGAS