Effective Error Estimates for Quasi-Monte-Carlo Computations

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CCS-3

See LANL Report LA-UR-01-1950
http://lib-www.lanl.gov/la-pubs/00367143.pdf

Traditional Monte-Carlo Uses Statistical Sampling

Test Integral

$$\theta = \int_0^1 f(\alpha) d\alpha$$

Monte-Carlo Estimate

$$\theta_{MC,N} = \frac{1}{N} \sum_{m=1}^{N} f(\zeta_m)$$

The ζ_m are randomly sampled from the uniform distribution on (0,1).

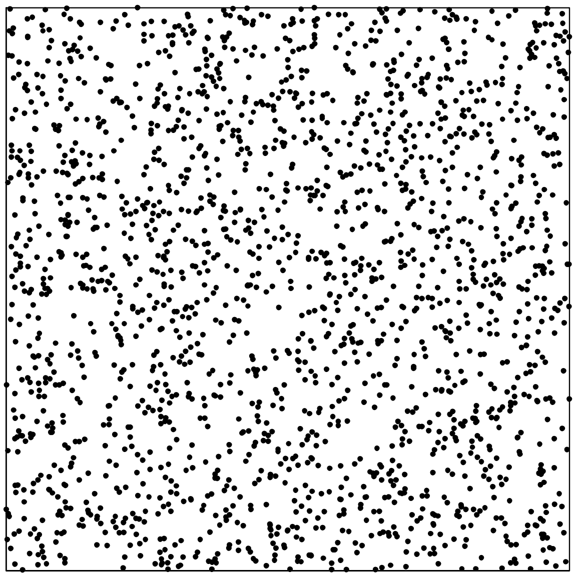
Errors may be estimated by computing square root of the sample variance.

$$s_{MC,N}^2 = \frac{1}{N(N-1)} \sum_{m=1}^{N} \left(f(\zeta_m) - \theta_{MC,N} \right)^2$$

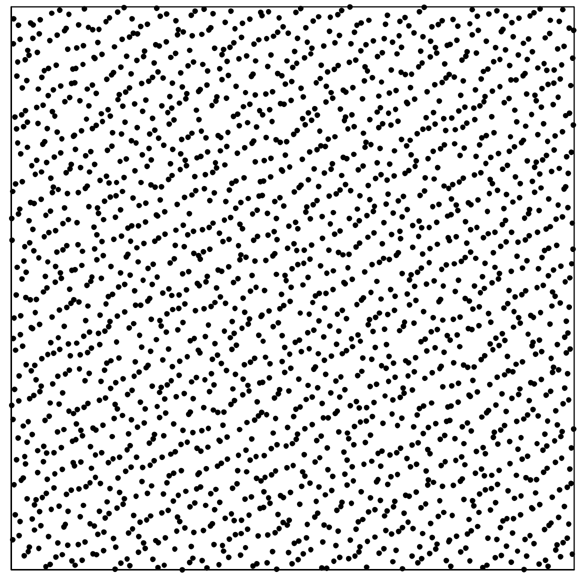
$$s_{MC,N} = \sqrt{s_{MC,N}^2}$$

Quasi-Monte-Carlo Uses Low-Discrepancy Points
Also called Quasi-Random Sequences

Random



Quasi-Random



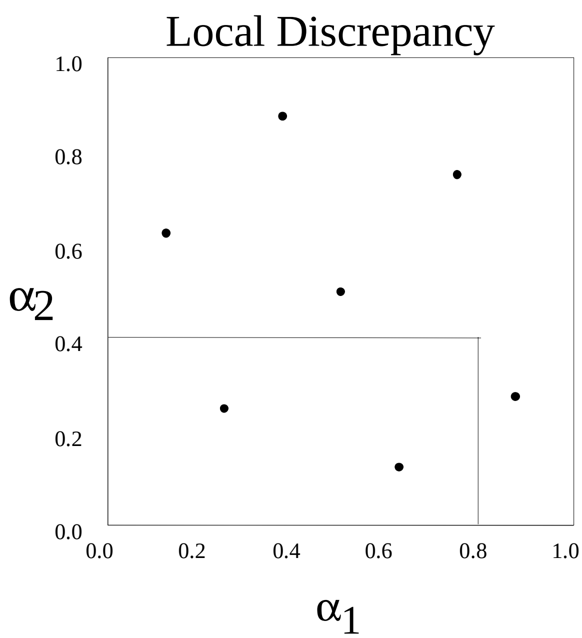
Quasi-Monte-Carlo Estimate

$$\theta_{QMC,N} = \frac{1}{N} \sum_{m=1}^{N} f\left(x_m\right)$$

The x_m are uniformly sampled on (0,1).

There is no analogue of the variance-type error estimate for Quasi-Monte-Carlo.

Measures of Irregularities of Distribution



The local discrepancy at a point α is given by:

$$\Delta(\alpha)=\frac{\nu(\alpha)}{N}-\mu(\alpha)$$

Where ν(α) is the number of points in the box delimited by the origin and α and μ(α) is the size of the box.

Global measures of distributional irregularity

$$D_N(X) = \sup_{\alpha \in U^k} |\Delta(\alpha)|$$

$$T_N(X) = \left(\int_{U^k} |\Delta(\alpha)|^2 \, d\mu(\alpha) \right)^{\frac{1}{2}}$$

Quasi-Random sequences can be constructed with:

$$D_N(X) \le c_k \frac{\ln(N)^k}{N}$$

$$T_N(X) \le c_k \frac{\ln(N)^{\frac{k-1}{2}}}{N}$$

Error Bounds for Quasi-Monte-Carlo

$$\left| \int_{U^k} f(\alpha)\, d\alpha - \frac{1}{N}\sum_{m=1}^{N} f(x_m) \right| \leq V(f) \cdot D_N(X)$$

V*(f)* is the Hardy & Krause variation of *f*.

$$\left| \int_{U^k} f(\alpha)\, d\alpha - \frac{1}{N}\sum_{m=1}^{N} f(x_m) \right| \leq \left(\int_{U^k} \left(\frac{\partial^k}{\partial \alpha_1 \ldots \partial \alpha_k} f(\alpha) \right)^2 d\mu(\alpha) \right)^{1/2} \cdot T_N(X) .$$

Lower Bounds on Discrepancy

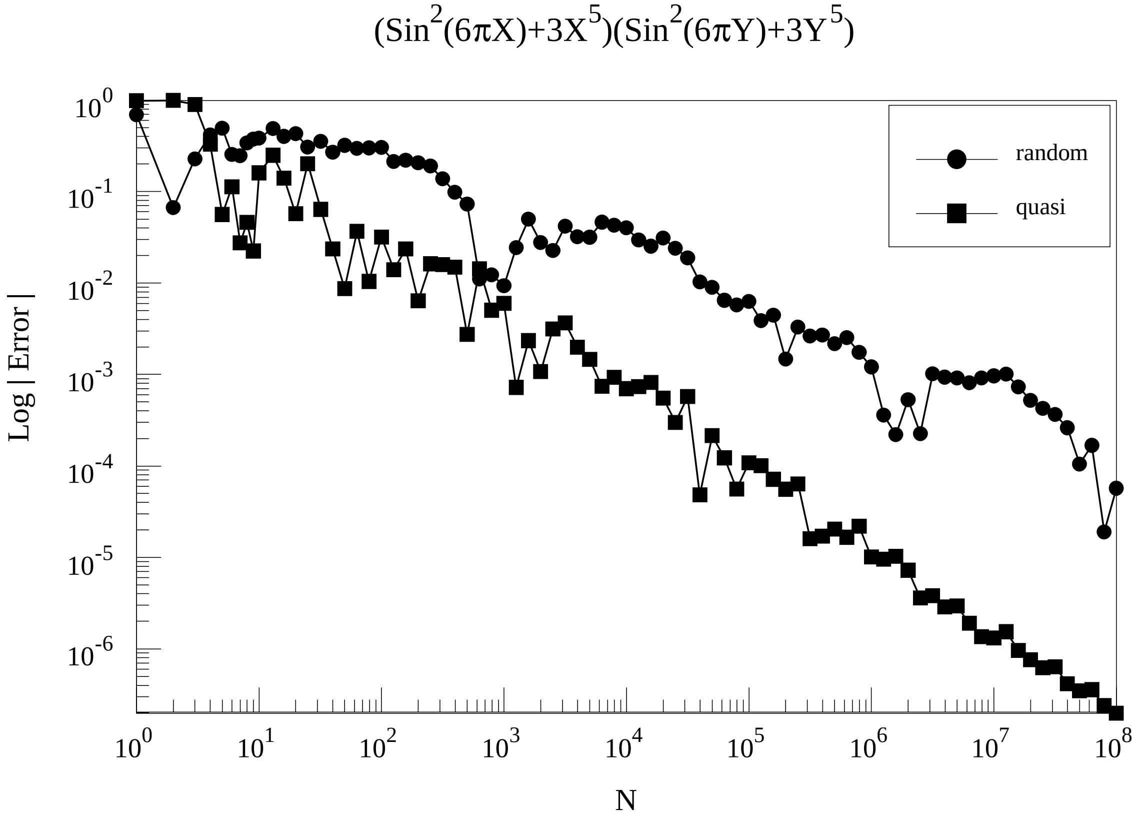
$$D_N(X) \geq c_k \frac{\ln(N)^{\frac{k-1}{2}}}{N}$$

$$T_N(X) \geq c_k \frac{\ln(N)^{\frac{k-1}{2}}}{N}$$

Discrepancy of a Random Sequence

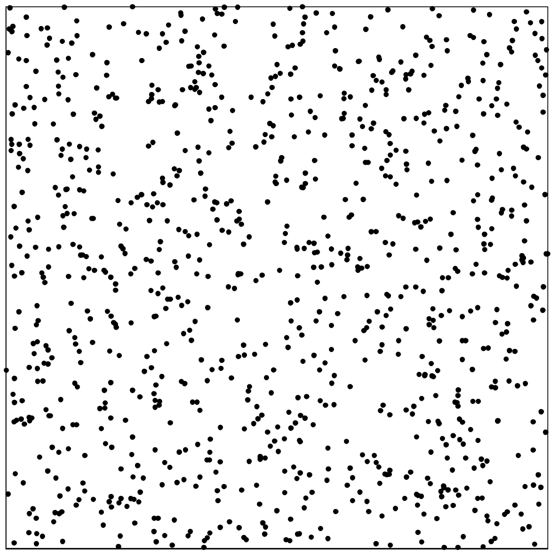
$$E(D_N(X)) = \sqrt{\frac{\ln(\ln(N))}{2\ N}}$$

$$E(T_N(X)) = \sqrt{\frac{1/2^k - 1/3^k}{N}}$$

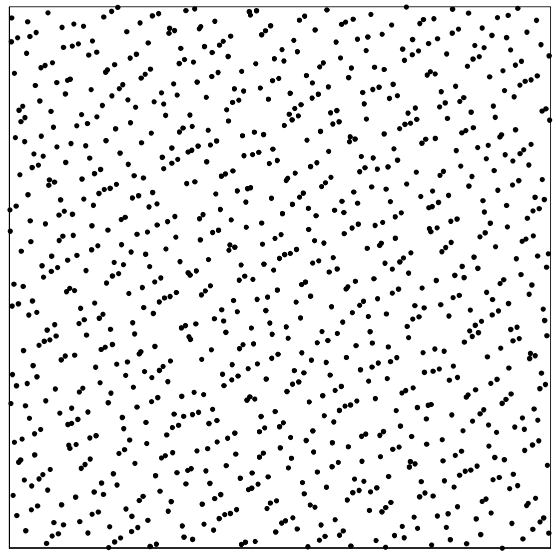


$(\mathrm{Sin}^2(6\pi X)+3X^5)(\mathrm{Sin}^2(6\pi Y)+3Y^5)$
random
quasi
Log | Error |
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^0 10^1 10^2 10^3 10^4 10^5 10^6 10^7 10^8
N

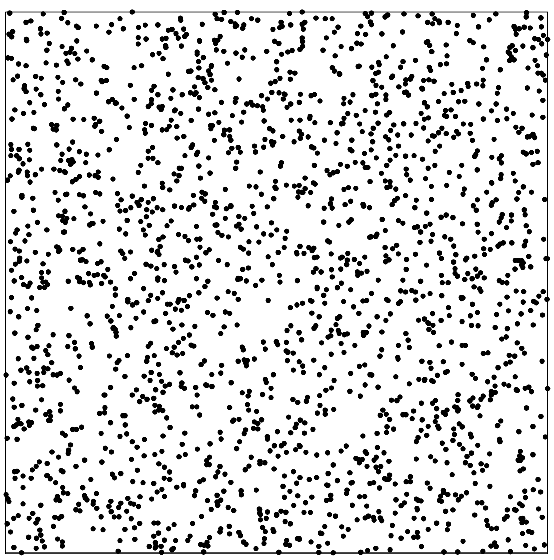
1000 Pseudo Random



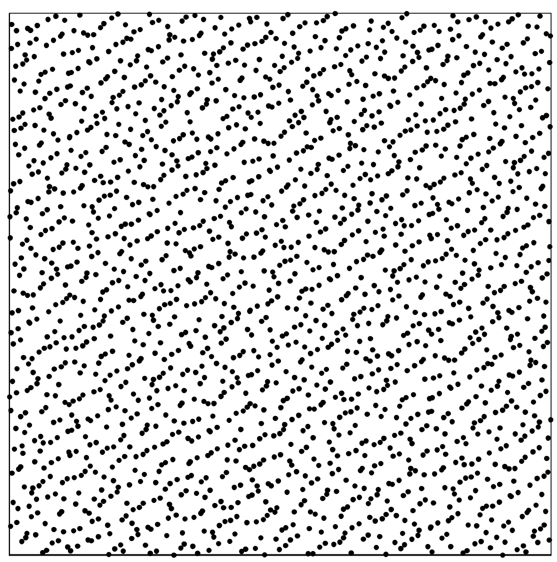
1000 Quasi Random



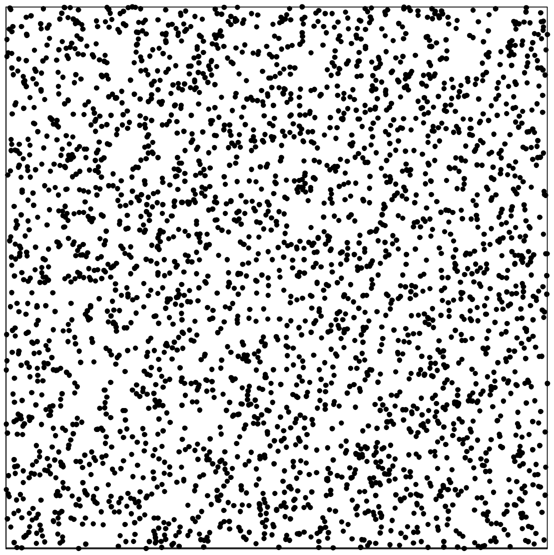
2000 Pseudo Random



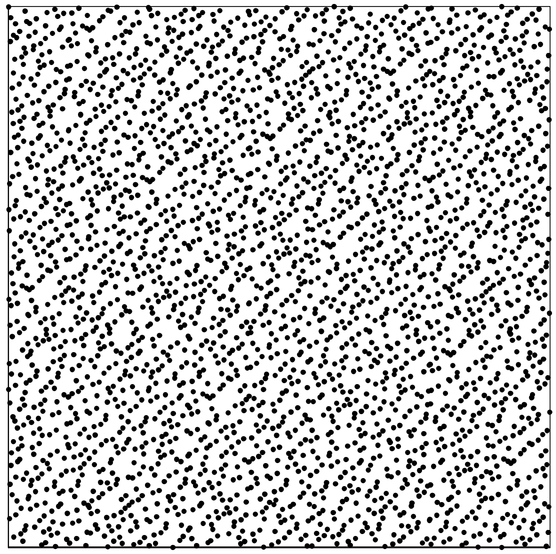
2000 Quasi Random



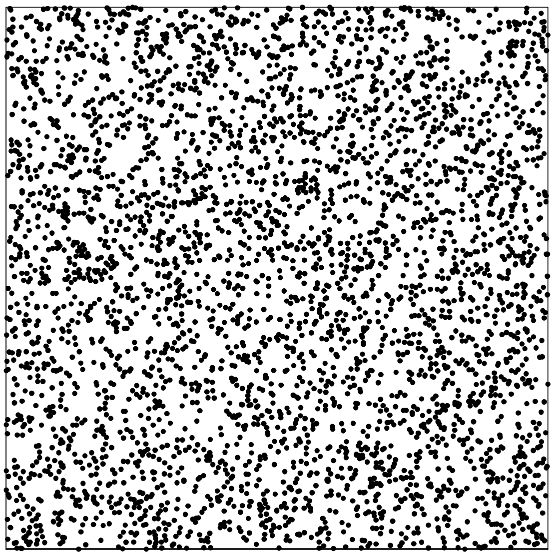
3000 Pseudo Random



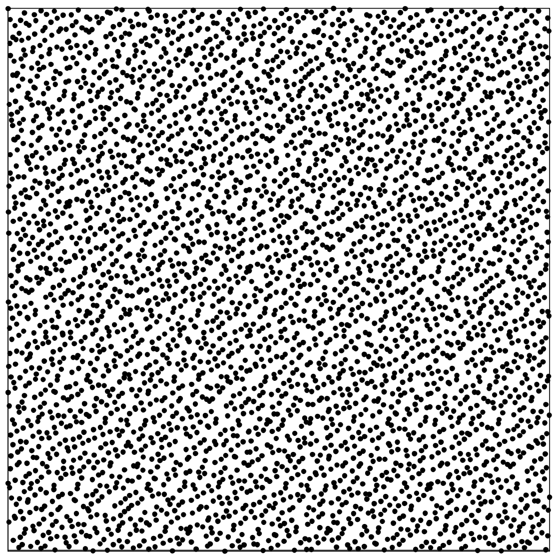
3000 Quasi Random



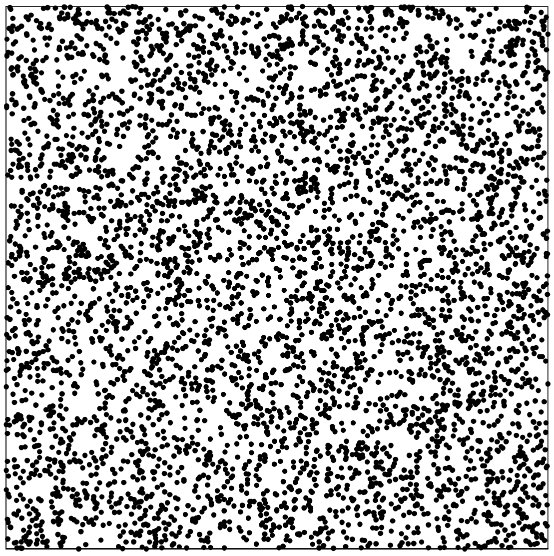
4000 Pseudo Random



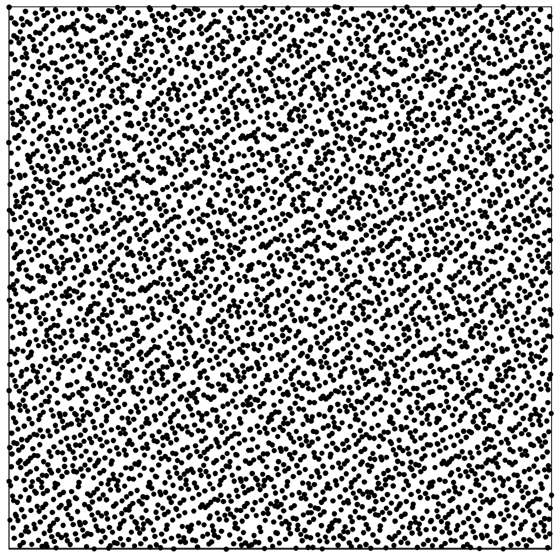
4000 Quasi Random



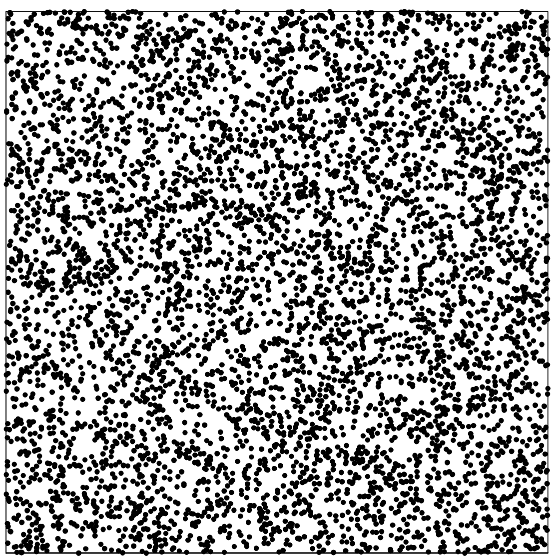
5000 Pseudo Random



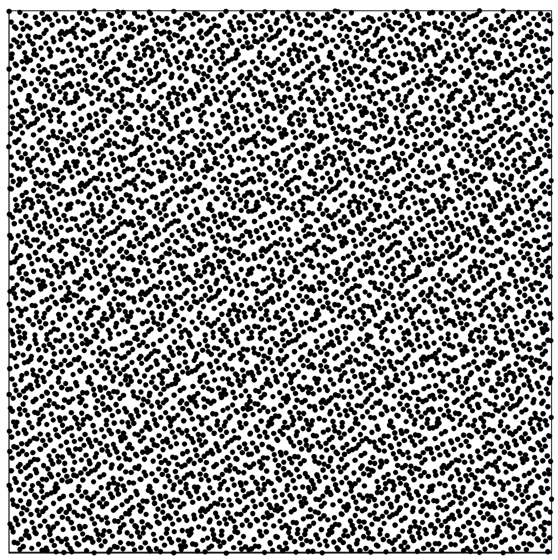
5000 Quasi Random



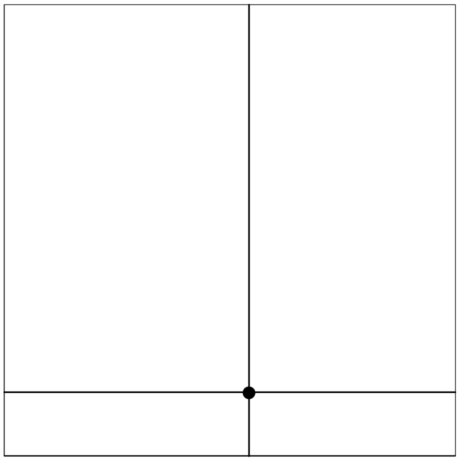
6000 Pseudo Random



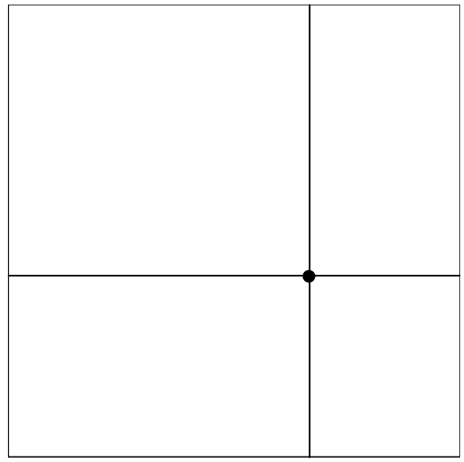
6000 Quasi Random



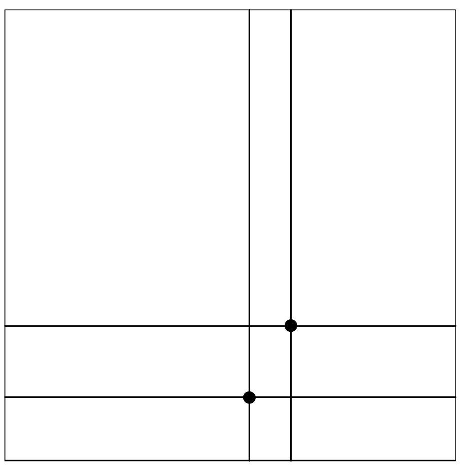
1 Pseudo Random



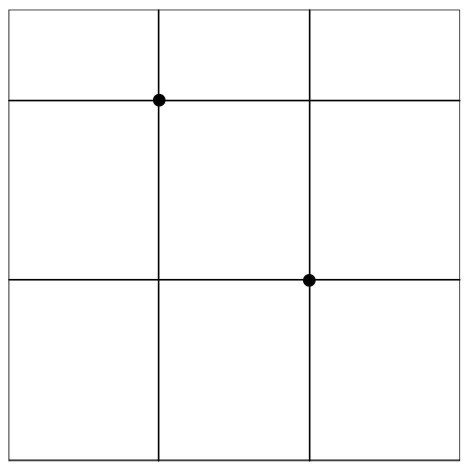
1 Quasi Random



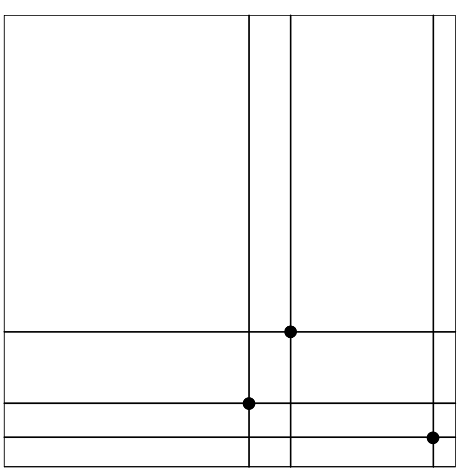
2 Pseudo Random



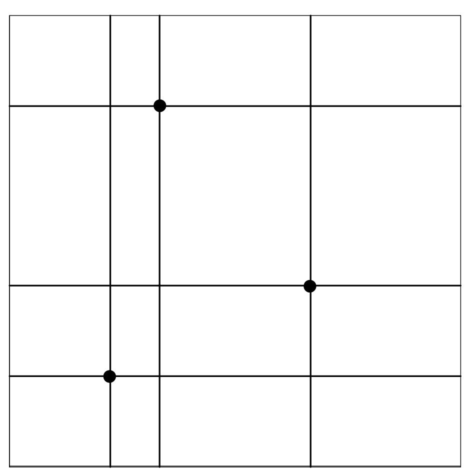
2 Quasi Random



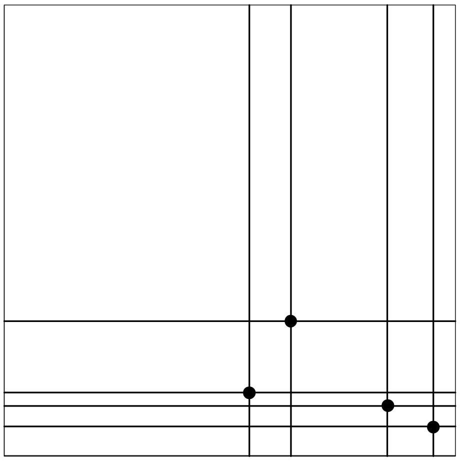
3 Pseudo Random



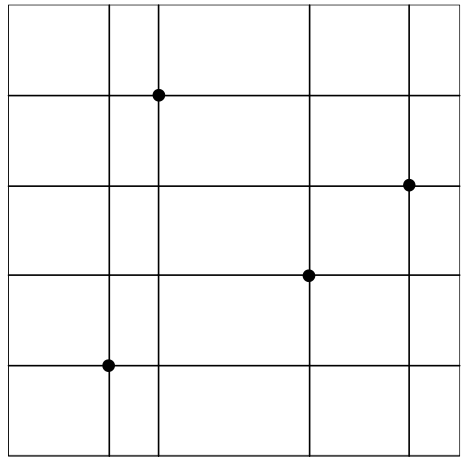
3 Quasi Random



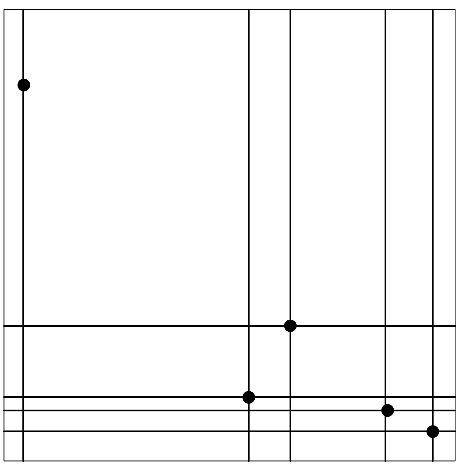
4 Pseudo Random



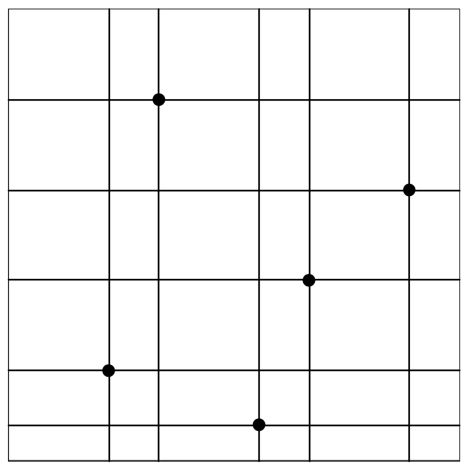
4 Quasi Random



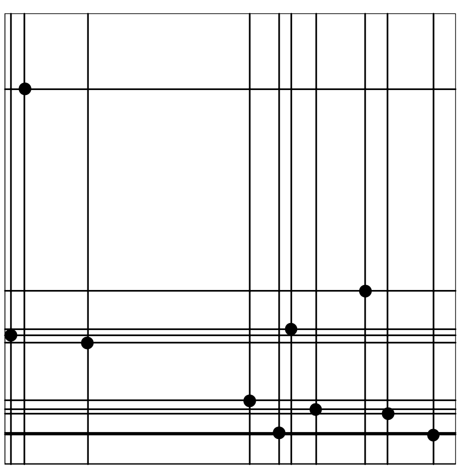
5 Pseudo Random



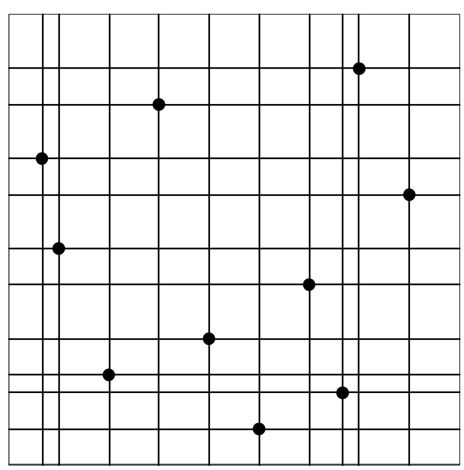
5 Quasi Random



10 Pseudo Random



10 Quasi Random



Some Low-Discrepancy Sequences

Fractional parts of multiples of square roots of primes.
Weyl, Richtmeyer

$$X_{N,i} = \{ N \sqrt{P_i} \}$$

As above but using square roots of square-free integers . Any set of irrationals, linearly independent over the rationals will suffice.

Halton Sequence. Digit Reversal

$$if \; N = \sum_{j=1}^{\infty} a_j \, P^j$$

$$then \; \phi_P(N) = \sum_{j=1}^{\infty} a_j \, P^{-j-1}$$

Warnock's modification of the Halton Sequence

$$if\ N = \sum_{j=1}^{\infty} a_j P^j$$

$$then\ \omega_P(N) = \sum_{j=1}^{\infty} \left(a_j S_P\right) \mathrm{mod}\left(P\right) P^{-j-1}$$

$$X_U = \lceil P\{\sqrt{P}\}\rceil$$

$$X_L = \lfloor P\{\sqrt{P}\}\rfloor$$

$$\frac{X_U}{P} = \backslash d_1, d_2, d_3 \cdots d_k \backslash$$

$$\frac{X_L}{P} = \backslash e_1, e_2, e_3 \cdots e_m \backslash$$

Choose S_P as either X_U or X_L according to:

1. The smaller sum or partial quotients.
2. The smallest largest partial quotient.
3. The nearest to fractional part of the square root of P.

Error Estimate

The empirical distribution function of a of a low-discrepancy sequence in, for example, 3 dimensions converges to the distribution function of a 3-dimensional uniform distribution.

The projections of coordinate values converge to the distribution functions of 3 independent 1-dimensional uniform distributions.

Three 1-dimensional quasi-Monte-Carlo estimates are made using the coordinate values and these estimates treated as independent samples. The variance of these estimates is used as the estimate of the integration error.

Taking the sequences ω_3 , ω_5, and ω_7 would give the following samples:

N	ω_3	ω_5	ω_7
1	2/3	2/5	5/7
2	1/3	4/5	3/7
3	2/9	1/5	1/7
4	8/9	3/5	6/7
5	5/9	2/25	4/7
6	1/9	12/25	2/7
7	7/9	22/25	5/49
8	4/9	7/25	40/49

The ω sequences fill the 3-cube uniformly.
The averages of a function over ω_3 , ω_5 and ω_7 are used as 3 independent samples

Computational Method

For a 1-dimensional integral.

1 Choose a 5-dimensional quasi-random sequence.
2 Compute 5 QMC estimates of the integral using the coordinate values.
3 Compute the mean and standard deviation of the 5 estimates.

For the same amount of work, N samples,
R-dimensional sequence.

$$\varepsilon_{MC} = \frac{1}{\sqrt{RN}}$$

Traditional Monte-Carlo

$$\varepsilon_{QMC} = \frac{\ln(NR)}{NR}$$

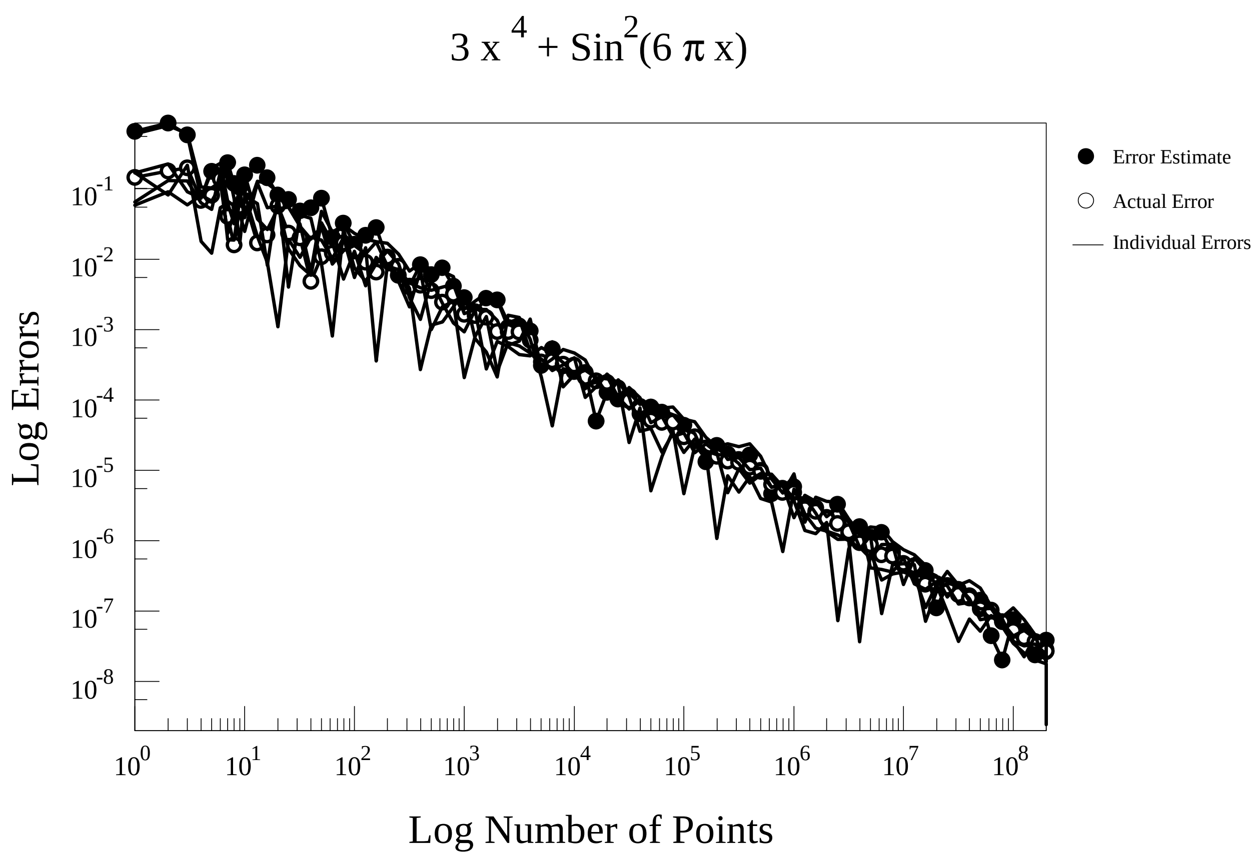
The usual QMC
No error estimate

$$\varepsilon_{NEW} = \frac{\ln N}{N\sqrt{R}}$$

With error estimate

Plot of errors from using the 5 coordinates of a 5-dimensional low-discrepancy sequence to estimate the integral of a 1-dimensional function.

The plot shows the actual errors of each estimate along with the error of the mean and the 99% confidence interval computed by using the variance over the 5 means.



Notes on Examples

The Traditional-Monte-Carlo computations use the linear-congruential pseudo-random number generator:

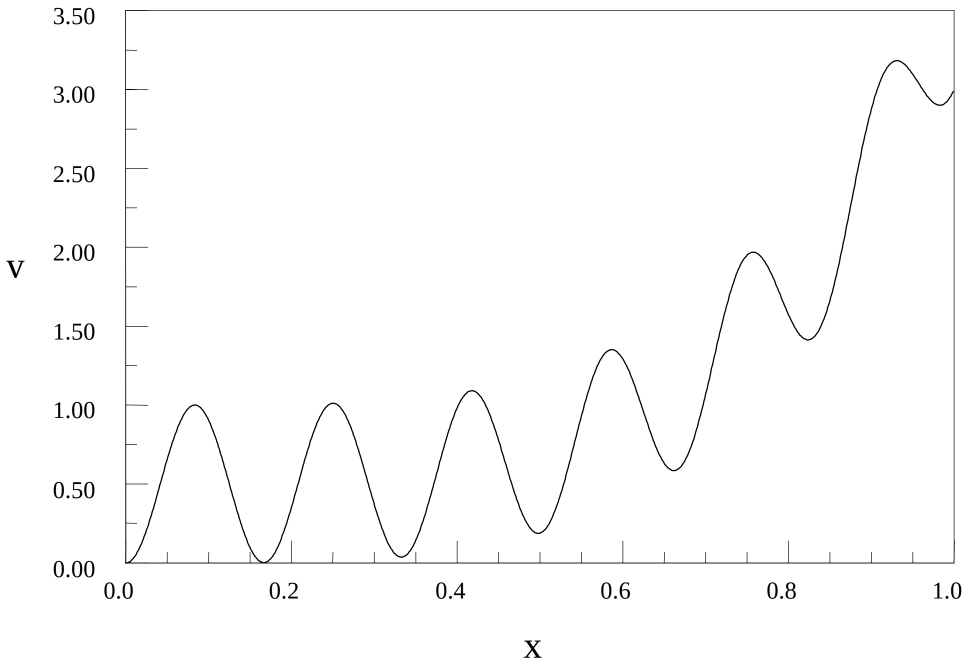
$$X_{i+1} = \left(6824416601091123613 \cdot X_i + 1\right) \bmod 2^{64}$$

$$X_0 = 3127516188341906279$$

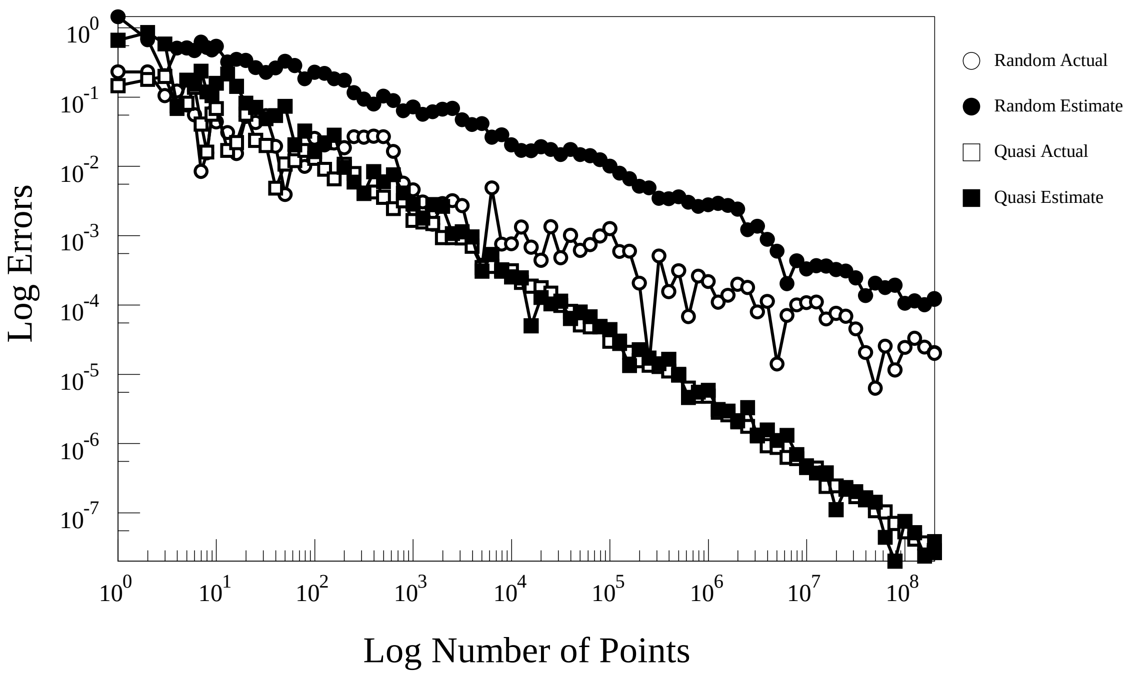
The quasi-Monte-Carlo computations use the sequences ω_3 , ω_5 , ω_7 , ω_{11} , ω_{13} .

The errors are reported as the 99% confidence interval from the t-density with 4 degrees of Freedom, 4.604 time the standard deviation.

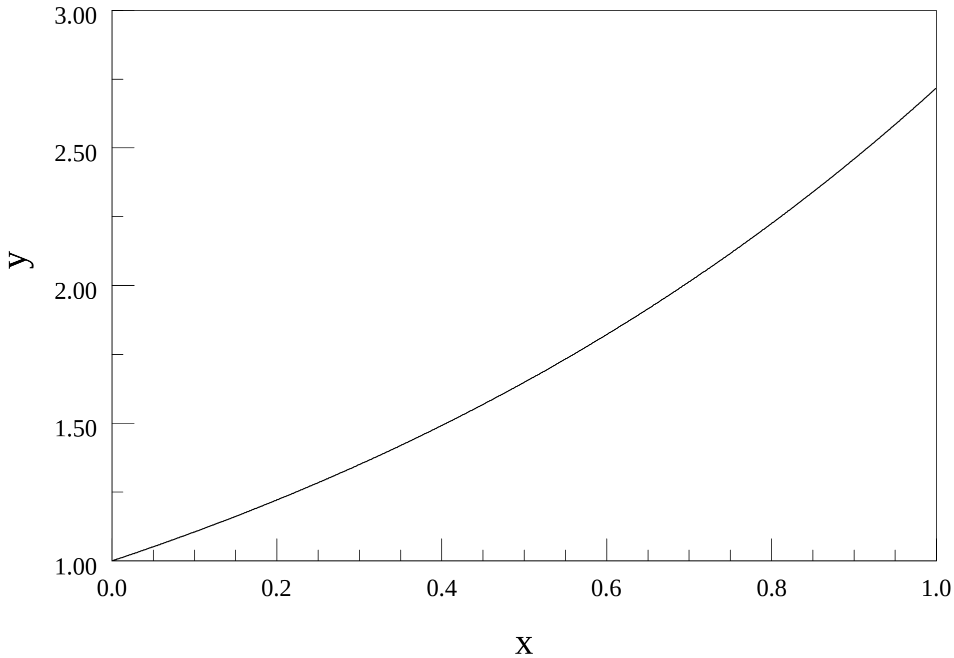
$3x^4 + \mathrm{Sin}^2(6\pi x)$



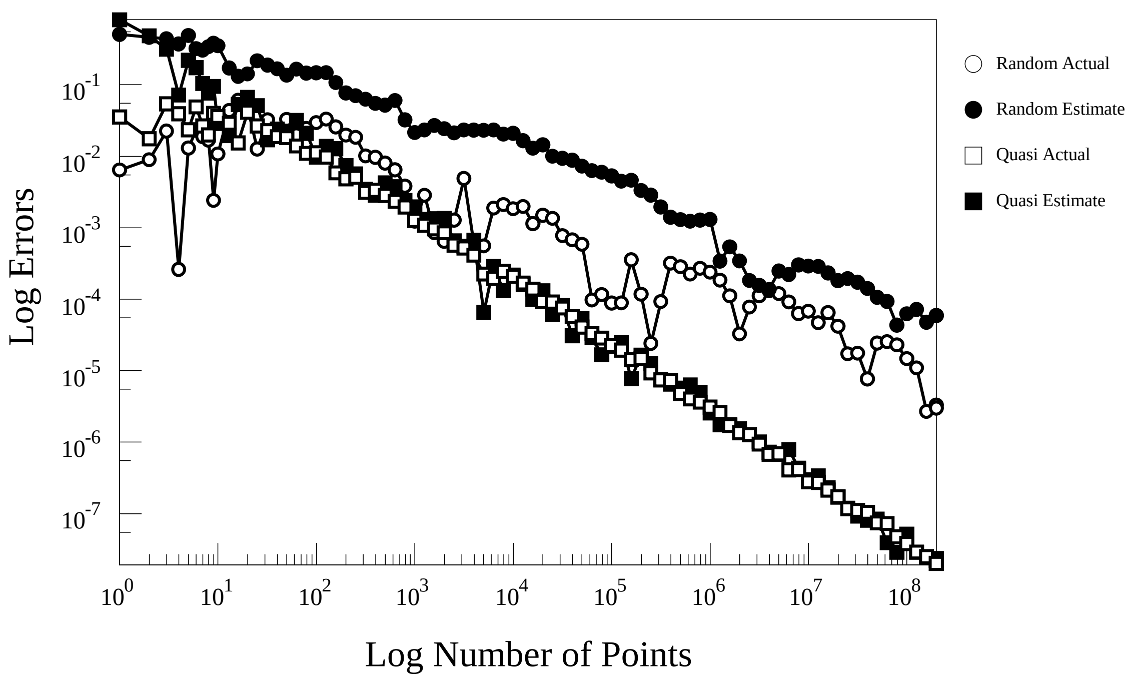
$3x^4 + \mathrm{Sin}^2(6\pi x)$



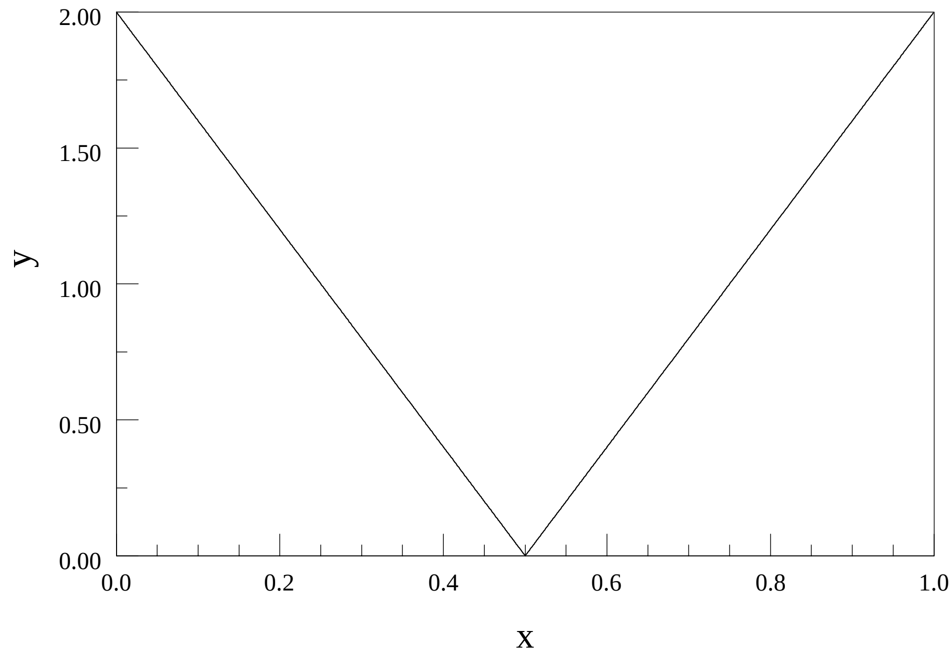
e^x


3.00
2.50
2.00
1.50
1.00
y
0.0
0.2
0.4
0.6
0.8
1.0
x

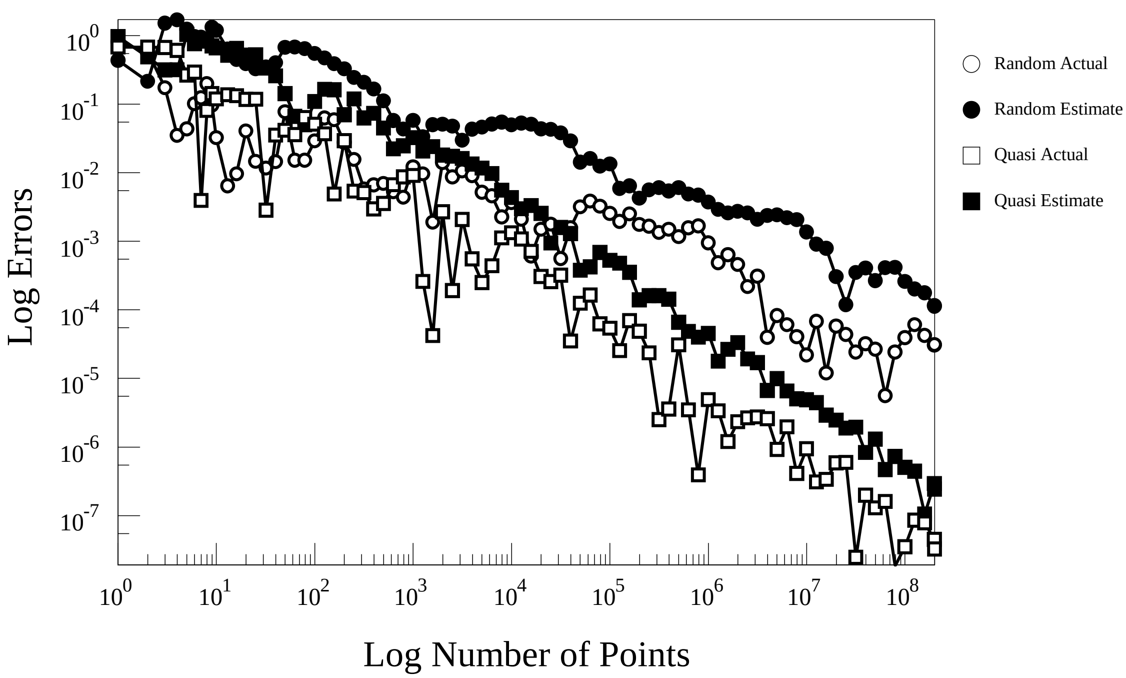
$e^x e^y/(e-1)^2$


Log Errors
10-1
10-2
10-3
10-4
10-5
10-6
10-7
100
101
102
103
104
105
106
107
108
Log Number of Points
Random Actual
Random Estimate
Quasi Actual
Quasi Estimate

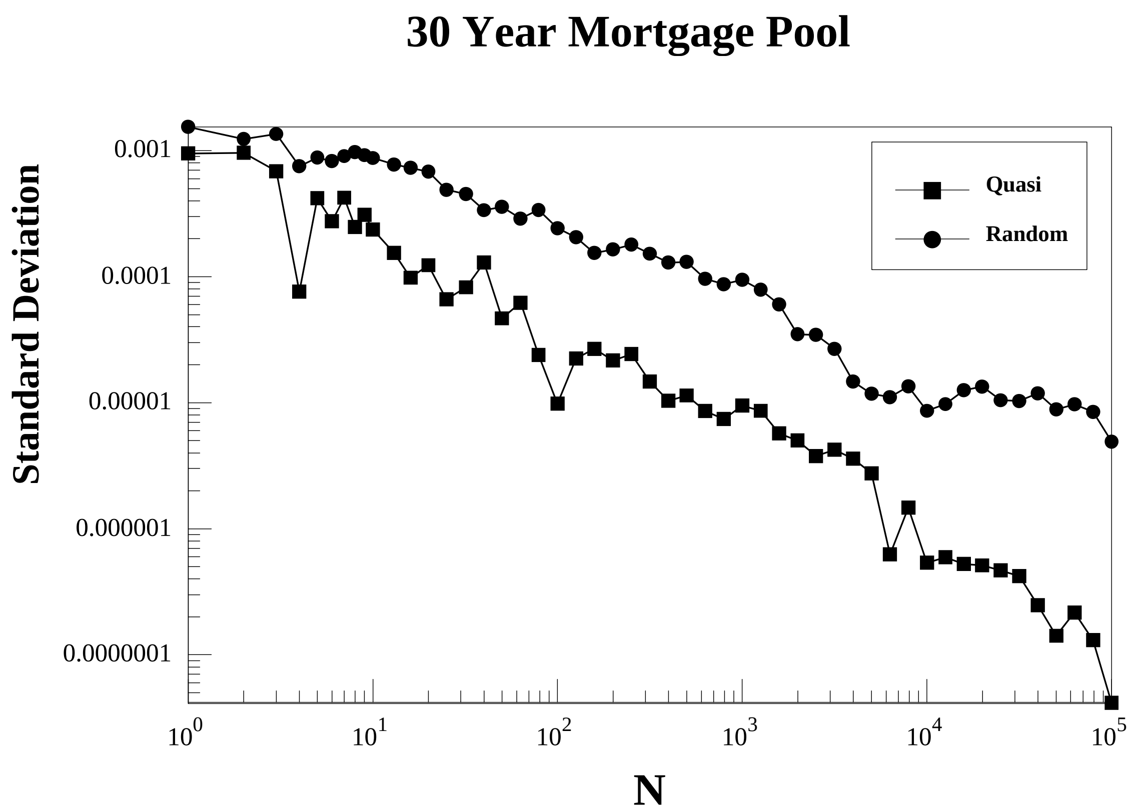
|4x-2|



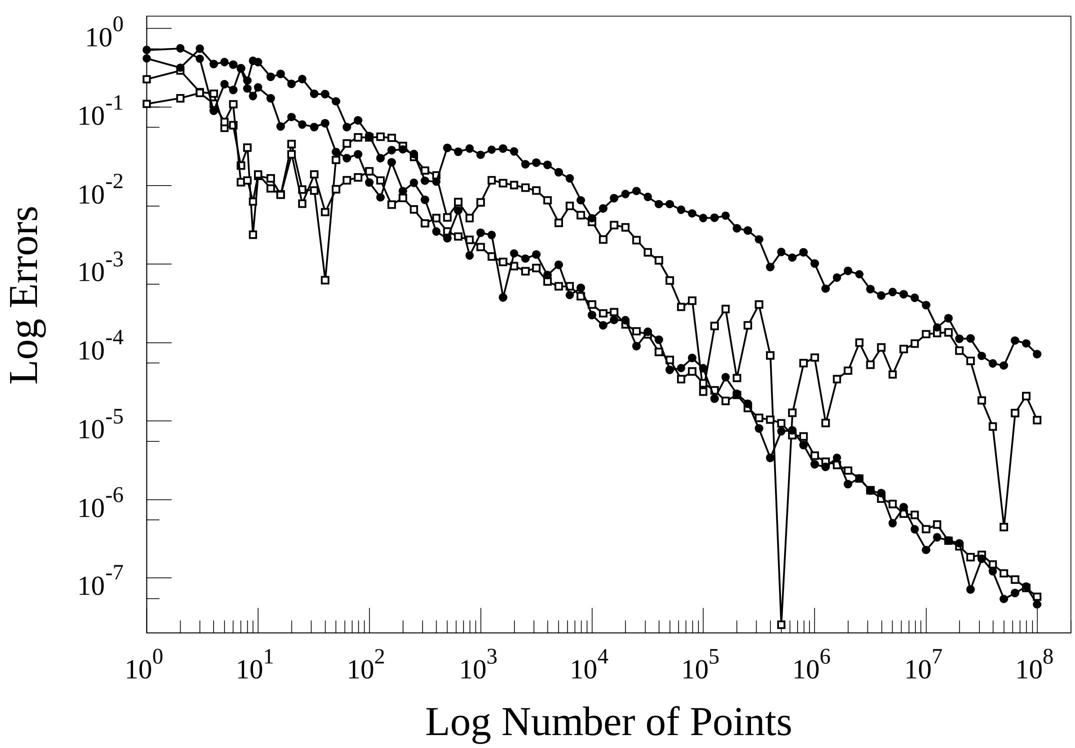
|(4w-1)(4x-2)(4y-2)(4z-2)|



A 360 month mortgage pool. Monte-Carlo and Quasi-Monte-Carlo estimates. Uses 1800 dimensional quasi-random sequence.



$(3 X^5 + \mathrm{Sin}^2(6 \pi X)+j)/(1+j)$ Product from j=1,15



Convergence Quadratic

A quadratic convergence can be obtained for periodic functions with a method of Niederreiter's.

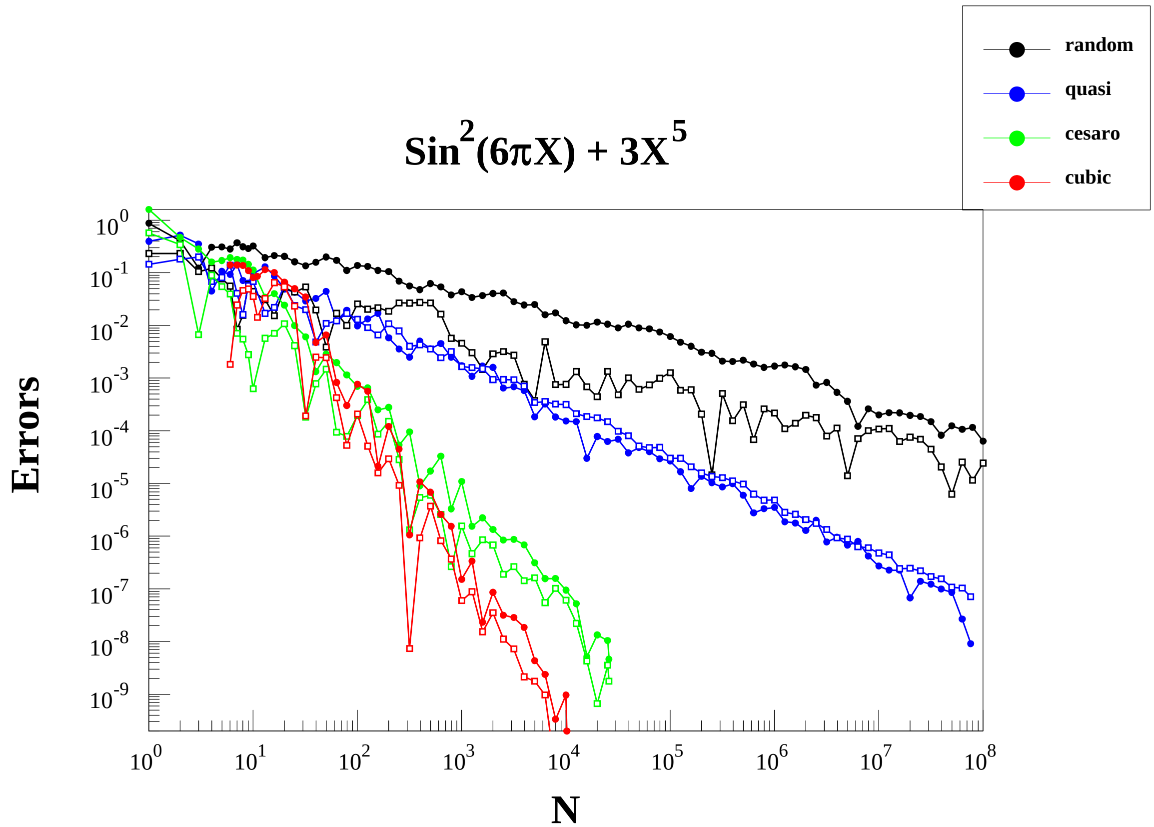
A modification of Césaro averaging of function values using the square roots of the primes seqence can give quadratic convergence.

$$\theta_{NQ} = \frac{1}{N^2} \sum_{m=1}^{2N-1} N - \left| N - m \right| f\left(x_m\right)$$

Errors may be estimated as described previously.
Non-periodic functions may be periodized by various periodizing transforms. Laurie's is:

$$f\left(x\right) \rightarrow f\left(g\left(x\right)\right) g'\left(x\right) dx$$

$$g\left(x\right) = 7x^3 - 21x^5 + 21x^6 - 6x^7$$



Cubic and higher-order convergence may be achieved with higher-order summations.