High-dimensional Numerical Integration: the Monte Carlo and Quasi Monte Carlo Ways

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Abstract

This research addresses high-dimensional numerical integration, which is complex and computationally intensive. Traditional methods are inefficient in high dimensions, so we use Monte Carlo methods with random sampling for scalability and Quasi-Monte Carlo methods with low-discrepancy sequences for better accuracy and faster convergence.

Estimation of integrals

We estimate the integral of the function

$$I(f) = \int_{[0,1]^s} f(x)\,dx \approx I_n(f) = \frac{1}{n}\sum_{k=0}^{n-1} f(x_k)$$

where $f : [0,1]^s \to \mathbf{R}$, x_k are samples on $[0,1]^s$, and n is the number of samples.

Rank-1 random shift lattice

Given the generating vector $z \in \mathbf{Z}^s$ and n independent random shifts $\Delta^{(i)}$ from the uniform distribution on $[0,1]^s$, then points of a rank-1 lattice with random shift are specified by

$$x_i = \frac{iz \ mod \ n}{n} + \Delta^{(i)} \in [0,1]^s$$

for $i = 0, 1, ..., n-1$.

Halton sequence

Given a positive value a and a prime number p, a can be expressed in a base p with a sequence of digits

$$d_m(a)...d_2(a)d_1(a)$$

where $0 \le d_i(a) \le p-1 \ \forall i$.

Then the halton sequence points base on p are constructed by

$$\phi_p(a) = 0.d_1(a)d_2(a)...d_m(a).$$

Sobol sequence

Choose a primitive polynomial of some degree s_j in the field Z_2,

$$x^{s_j} + a_{1,j}x^{s_j-1} + a_{2,j}x^{s_j-2} + ... + a_{s_j-1,j}x + 1$$

where the coefficients are either 0 or 1.

Define a sequence of positive integers $\{m_{1,j}, m_{2,j}, ...\}$ by the recurrence relation

$$m_{k,j} = 2a_{1,j}m_{k-1,j} \oplus 2^2 a_{2,j} m_{k-2,j} \oplus ... \oplus m_{k-s_j,j}$$

where $\oplus$ is bitwise exclusive-or operator and the initial value can be chosen freely with $m_{k,j}, 1 \le k \le s_j$, is odd and less than 2^k.

The direction number $\{v_{1,j}, v_{2,j}, ...\}$ are defined by

$$v_{k,j} = \frac{m_{kj}}{2^k}.$$

Then $x_{i,j}$, the j-th component of the ith point in a Sobol sequence, is given by

$$x_{i,j} = i_1 v_{1,j} \oplus i_2 v_{2,j} \oplus ...$$

where i_k is the kth digit from the right when i is written in binary $i = (...i_3 i_2 i_1)_2$.

Error bound for random shift lattice rule

Assume that the integrand f belongs to a weighted Sobolev space of functions whose mixed first derivatives are square-integrable, with the norm given by

$$\|f\|_\gamma^2 = \sum_{u \subseteq \{1,\ldots,s\}} \frac{1}{\gamma_u} \int_{[0,1]^{|u|}} \left(\int_{[0,1]^{s-|u|}} \frac{\partial^{|u|} f}{\partial x_u}(x)\,dx_{-u} \right)^2 dx_u.$$

For a randomly shifted lattice rule, we have the root-mean-square error bound

$$\sqrt{\mathbf{E}|I(f) - I_n(f)|^2} \le e_\gamma^{sh}(z)\|f\|_\gamma = \sqrt{\int_{[0,1]^s} \left(\underset{\|f\|_\gamma \le 1}{sup} |I(f) - I_n(f)| \right)^2 d\Delta} \ \ \|f\|_\gamma.$$

Theorem

A lattice rule in dimension s can be constructed such that the worst case error

$$e_\gamma^{sh}(z) \le \left(\frac{1}{|\mathbf{U}_n|} \sum_{\emptyset \ne u \subseteq \{1,\ldots,s\}} \gamma_u^\lambda \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda} \right)^{|u|} \right)^{1/(2\lambda)}$$

for all $\lambda \in (1/2, 1]$, where $\zeta(x) = \sum_{k=1}^\infty k^{-k}$ is the Riemann zeta function, $|\mathbf{U}_n| = n-1$ when n is prime, $|\mathbf{U}_n| = n/2$ when n is a power of 2, and $|\mathbf{U}_n| \le n/2$ is a power of a prime.

Error bound analysis

Consider $f(x) = exp(c\sum_{j=1}^s)x_j j^{-b}$, $x \in \mathbf{R}^s$, with constants $c > 0, b \ge 0$.

Let us assume that $\|f\|_\infty \le C_{c,b,s}$, then by theorem, if n is a power of a prime ,then we obtain

$$\mathbf{E}|I(f) - I_n(f)|^2 \le \frac{C_{c,b,s}^2}{n^{1/\lambda}} \left(2 \sum_{\emptyset \ne u \subseteq \{1,\ldots,s\}} \gamma_u^\lambda \left(\frac{2\zeta(2\lambda)}{(2\pi^2)^\lambda} \right)^{|u|} \right)^{(1/\lambda)} \left(\sum_{u \subseteq \{1,\ldots,s\}} \frac{1}{\gamma_u} \prod_{j \in u} (c^2 j^{-2b}) \right).$$

The upper bound is minimized by choosing

$$\gamma_u = \prod_{j \in u} \left(\frac{(2\pi^2)^\lambda}{2\zeta(2\lambda)} c^2 j^{-2b} \right)^{1/(1+\lambda)}.$$

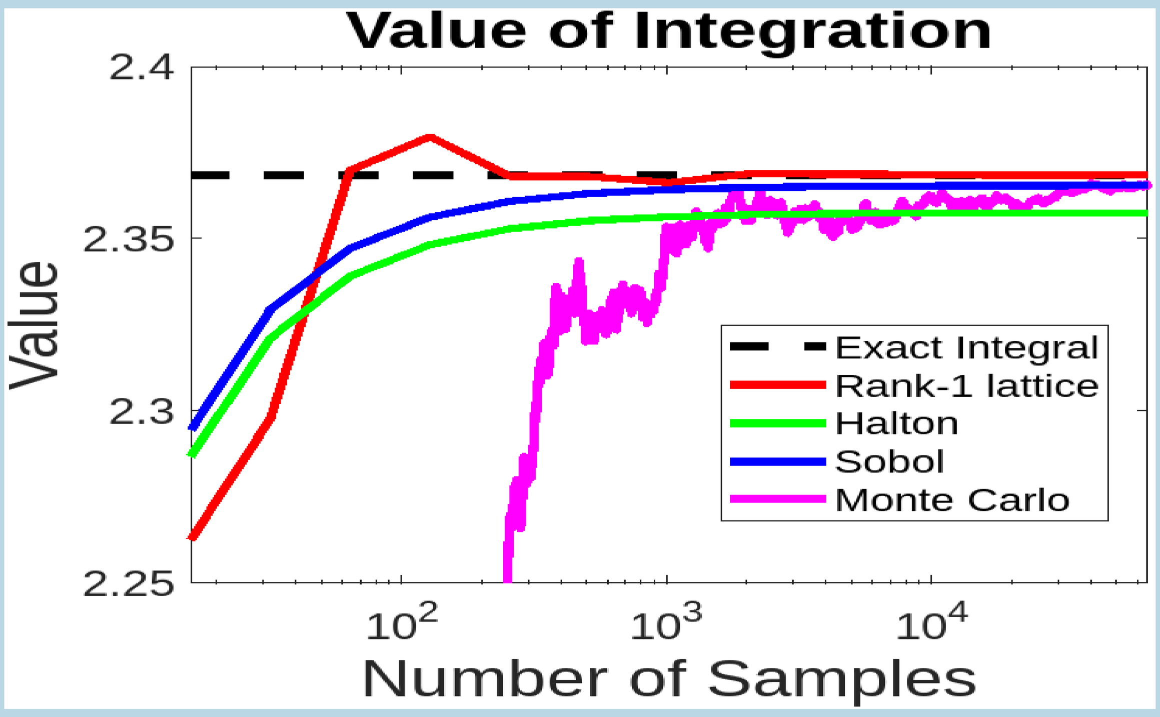
We take $\lambda \to 1/2$ the more our root-mean-square error bound will tell us we have $1/n$ convergence. However $\zeta(2\lambda) = \infty$ and the bound blows up. In light of the above analysis, we consider product weights of the form

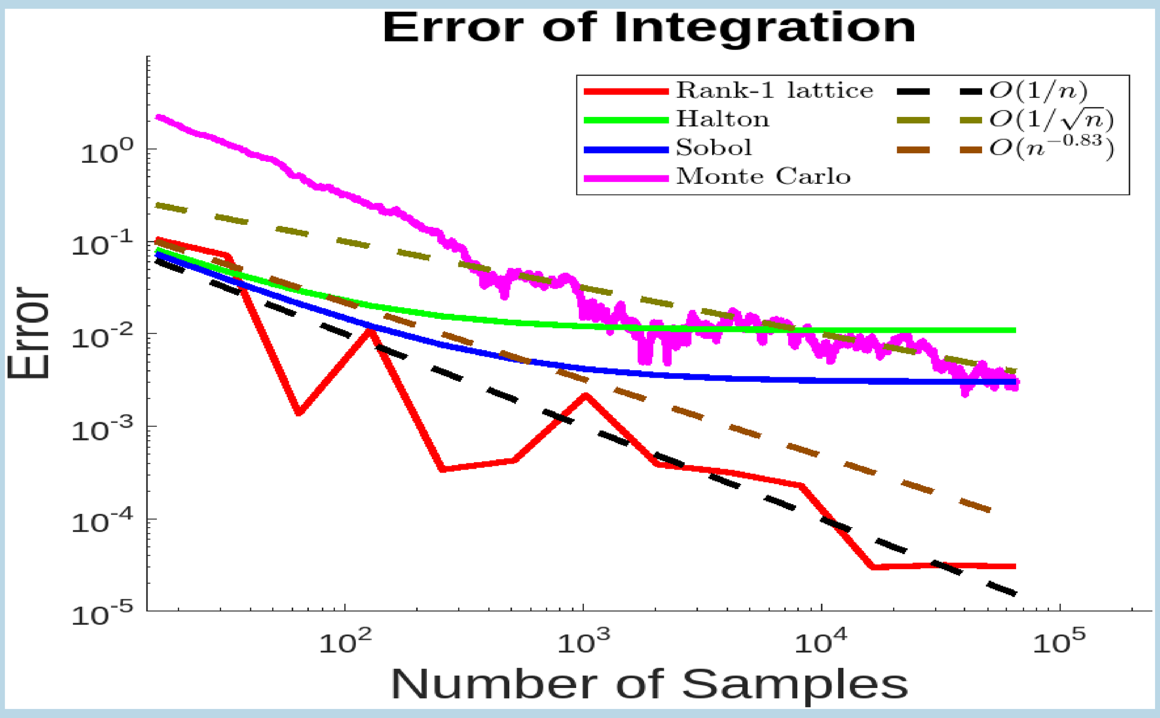
$$\gamma_j = \left(\frac{cj^{-b}}{\sqrt{2}} \right)^{1.25}.$$

The theory then indicates that we get around $O(n^{-0.83})$ convergence.

Results of numerical integration tests

The following graphs show the integration value and error for above function f with $c = 1, b = 2$.





Conclusion

Among the four types of sampling sequences, using the rank-1 random shift lattice sequence achieves the best results and converges rapidly.

References

[1] S. Joe and F. Y. Kuo, Notes on generating Sobol' sequences (2008).

[2] F. Y. Kuo and D. Nuyens, A Practical Guide to Quasi-Monte Carlo Methods (2016).