On the Weighted Star Discrepancy of Lattice Rules

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Acknowledgements

Many of the results reported in this talk have been developed as joint work with *Stephen Joe* and *Pierre L'Ecuyer*.

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Outline

- The weighted star discrepancy
- Bounds on the weighted star discrepancy of lattice rules
- Approach and results
- Tractability issues
- Conclusions

Multivariate integrals

High dimensional integrals of the form

$$I_d(f) = \int_{[0,1]^d} f(\mathbf{x}) \mathrm{d}\mathbf{x}$$

can be approximated by quadrature rules given by

$$Q_{n,d}(f) = \frac{1}{n} \sum_{k=0}^{n-1} f\left(\mathbf{x}_k\right),$$

where the point set $P_n := \{\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_{n-1}\} \subseteq [0,1]^d$ may be produced randomly (Monte Carlo) or in some deterministic manner (quasi-Monte Carlo).

QMC methods

To improve the convergence produced by Monte Carlo, one has to select points that have a **high uniformity** over the unit cube. This high uniformity may be understood with respect to several measures of goodness, which are broadly referred to as **"discrepancies"**.

We say that a point set P_n is **uniformly distributed** over the unit cube it its **discrepancy** goes to 0 as $n \to \infty$.

There are QMC point sets whose discrepancy is $O(n^{-1}(\ln n)^d)$ - better than MC but the involved constant can be large if the dimension d is large - the "**curse of dimensionality**".

In many applications, it has been noticed that the **effective dimension** of the problem is lower than its real dimension. This is explained by the fact that variables or groups of variables have different importance.

Weights were introduced to reflect the different importance of variables (Sloan and Woźniakowki). Consequently, theory had to be developed for weighted figures of merit, such as the **weighted star discrepancy** (definition to follow).

There exist lattice rules such that convergence for weighted figures of merit is $O(n^{-1+\delta})$ or $O(n^{-\alpha+\delta})$ for any $\delta > 0$, where $\alpha > 1$ and with the involved constant independent of the dimension.

Quadrature error

The quadrature error can be bounded by the product of two quantities: one depending on the point-set (the discrepancy) and the second one depending on the integrand (variation of the function).

$$|Q_{n,d}(f) - I_d(f)| \leq D_{p,\gamma}(P_n) \cdot V_q(f),$$

where $p, q \geq 1$ with $1/p + 1/q = 1$.

A popular framework is given by RKHS and L_2-type discrepancies.

Weighted star discrepancy

The weighted star discrepancy is based on an L_∞ norm and fits this framework. Indeed, from Zaremba's identity and Hölder's inequality, it follows that

$$|Q_{n,d}(f) - I_d(f)| \leq \max_{\mathfrak{u}\subseteq\mathcal{D}} \sup_{\mathbf{x}_\mathfrak{u}\in[0,1]^{|u|}} \gamma_\mathfrak{u} \left|\mathrm{discr}((\mathbf{x}_\mathfrak{u}, \mathbf{1}), P_n)\right| \times \sum_{\emptyset\neq\mathfrak{u}\subseteq\mathcal{D}} \gamma_\mathfrak{u}^{-1} \int_{[0,1]^{|\mathfrak{u}|}} \left| \frac{\partial^{|\mathfrak{u}|}}{\partial \mathbf{x}_\mathfrak{u}} f(\mathbf{x}_\mathfrak{u}, \mathbf{1}) \right| \mathrm{d}\mathbf{x}_\mathfrak{u},$$

where $\gamma_\mathfrak{u}$ is the weight associated with the set $\mathfrak{u} \subseteq \mathcal{D} := \{1, 2, \ldots, d-1, d\}$
This leads to a weighted star discrepancy $D^*_{n,\gamma}(\mathbf{z})$ given by

$$D^*_\gamma(P_n) := \max_{\mathfrak{u}\subseteq\mathcal{D}} \gamma_\mathfrak{u} \sup_{\mathbf{x}_\mathfrak{u}\in[0,1]^{|u|}} \left|\mathrm{discr}((\mathbf{x}_\mathfrak{u}, \mathbf{1}), P_n)\right|.$$

Discrepancy

The **local discrepancy** is defined by

$$\mathrm{discr}(\mathbf{x}, P_n) := \frac{|P_n(\mathbf{z}) \cap [\mathbf{0}, \mathbf{x})|}{n} - \mathrm{Vol}([\mathbf{0}, \mathbf{x})),$$

.

Discrepancies

The "classical" (unweighted) **star discrepancy** of a d-dimensional point set P_n is defined as

$$D^*(P_n) := \sup_{\mathbf{x} \in [0,1]^d} |\text{discr}(\mathbf{x}, P_n)|,$$

where $\text{discr}(\mathbf{x}, P_n)$ is the local discrepancy defined earlier.

Early theory in: H. Niederreiter - "Random Number Generation and Quasi-Monte Carlo Methods" (1992) and I.H. Sloan and S. Joe - "Lattice Methods for Multiple Integration" (1994).

It is known that there exist point sets such that the star discrepancy converges as $O(n^{-1}(\ln n)^d)$ - conjectureed to be the best possible. A refined convergence rate (mentioned earlier) can be obtained for the weighted star discrepancy.

Computing the weighted star discrepancy

Calculating the star discrepancy of a point set is an *NP*-hard problem (Gnewuch et al. 2008). Algorithms of a relative simple form have been proposed long ago, but all require $O(n^d)$ operations. Instead one prefers to use upper bounds on the weighted star discrepancy and then construct point sets that are "good".

Here we consider the weighted star discrepancy of lattice rules.

We prove that there exist lattice rules such that $D^*_\gamma(P_n) = O(n^{-1+\delta})$ for any $\delta > 0$, and with the involved constant independent of the dimension. There also are construction schemes available.

Rank-1 lattice rules

Are quadrature rules of the form

$$Q_{n,d}(f) = \frac{1}{n}\sum_{k=0}^{n-1} f\left(\left\{\frac{k\mathbf{z}}{n}\right\}\right),$$

where $\mathbf{z}$ is the "generating vector" of the lattice rule.

Usually, the generating vector is restricted to the set $\mathcal{Z}_n^d$, where $\mathcal{Z}_n := \{z : z \in \{1, 2, \ldots, n-1\},\ \gcd(z, n) = 1\}$. The number of elements of the set $\mathcal{Z}_n$ is given by $|\mathcal{Z}_n| = \varphi(n)$, where φ is Euler's totient function.

Shifted rank-$\mathbf{1}$ lattice rules

Are quadrature rules given by

$$Q_{n,d}(f) = \frac{1}{n}\sum_{k=0}^{n-1} f\left(\left\{\frac{k\mathbf{z}}{n} + \boldsymbol{\Delta}\right\}\right),$$

where $\boldsymbol{\Delta}$ is the "shift".

These shifted lattice rules preserve the geometrical structure of the point set and also allow randomisation.

Why consider this L_∞ version of the weighted star discrepancy?

- It requires lesser smoothness assumptions on the integrand than other types of L_p discrepancies. We need the integrand to have integrable partial mixed first derivatives.
- No requirement for periodicity.
- No need for a reproducing kernel.
- The weighted star discrepancy of lattice rules is invariant under shifts modulo 1.
- Results for subsequent L_p discrepancies can be obtained.

Observation

Theory on good lattice rules depends on:

1. The number of points, i.e. depending whether n is prime or not. Much easier to obtain results when n is prime.
2. The type of weights considered. Easier for product weights than for general weights.
3. The space of functions and the type of discrepancy considered.
4. The type of lattice rule considered (rank-1, shifted, higher rank).
5. The domain considered (bounded, unbounded).

Each assumption requires a separate analysis.

Approach - a very generic description

1. Selecting a figure of merit, depending on the integrands and the problems we want to solve.
2. Establishing bounds on the figure of merit, if needed.
3. Establishing existence results for good lattice rules, usually using an averaging argument *(If the average is good, then it must be a good one)*.
4. Then we turn to construction schemes such that the lattice rules constructed are not worse than the mean. One popular construction is the so-called **component-by-component (CBC)** construction (*details to follow*).
5. Computational aspects incurred by the construction (complexity, speeding up etc.)
6. Studying tractability problems - breaking the curse of dimensionality.

Assumptions

1. We assume functions have integrable partial mixed first derivatives.
2. We use the weighted star discrepancy as the figure of merit.
3. We assume weights are general (for tractability purposes, we assume weights are decreasing, i.e. the weight associated with a set cannot be bigger than the weight associated with any subset).
4. We assume n composite.
5. We assume lattice rules can be shifted arbitrarily.

This combination of assumptions has not been considered before. In particular, the combination of general weights and composite n is interesting.

Our approach

Consider the weighted star discrepancy given by

$$D^*_{n,\gamma}(\mathbf{z}) := \max_{\mathfrak{u}\subseteq\mathcal{D}} \gamma_{\mathfrak{u}} \sup_{\mathbf{x}_{\mathfrak{u}}\in[0,1]^{|u|}} \left|\mathrm{discr}((\mathbf{x}_{\mathfrak{u}},\mathbf{1}),P_n)\right|.$$

Establish bounds on the weighted star discrepancy.

$$D^*_{n,\gamma}(\mathbf{z}) \le \frac{1}{2} e_{n,d}(\mathbf{z}) + \max_{\mathfrak{u}\subseteq\mathcal{D}} \gamma_{\mathfrak{u}} \left(1 - \left(1 - \frac{1}{n}\right)^{|\mathfrak{u}|}\right),$$

where the expression of $e_{n,d}$ will be given next, while the second term is always $O(n^{-1})$.

General weights

When the weights are general, we have

$$e_{n,d}(\mathbf{z}) = \frac{1}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} \sum_{k=0}^{n-1} \prod_{j \in \mathfrak{u}} \left(\sum_{-n/2 < h \leq n/2}{}' \frac{e^{2\pi \mathrm{i} h k z_j / n}}{|h|} \right).$$

The $'$ at the sum indicates we omit the $h = 0$ term.

Earlier results were developed for product weights, that is $\gamma_{\mathfrak{u}} = \prod_{j \in \mathfrak{u}} \gamma_j$. This is easier to analyse.

Existence results

Are established by analysing a mean of the quantities $e_{n,d}(\mathbf{z})$ over all possible generating vectors. Such a mean is given by

$$M_{n,d,\gamma} := \frac{1}{\varphi(n)^d} \sum_{\mathbf{z} \in \mathcal{Z}_n^d} e_{n,d}(\mathbf{z}).$$

Recall that $\mathcal{Z}_n := \{z : z \in \{1, 2, \dots, n-1\}, \gcd(z, n) = 1\}$.

One can easily see that for n prime, we have $\varphi(n) = n - 1$.

Usual technique to establish the existence results

- Establish an expression for the mean or a bound.
- If such a bound is "good", then a "good" lattice rules does exist.

We proved that there exist and that we can construct lattice rules such that

$$e_{n,d}(\mathbf{z}) \leq \frac{2}{n} \sum_{\mathfrak{u} \subseteq \mathcal{D}} \gamma_{\mathfrak{u}} (c \ln n)^{|\mathfrak{u}|},$$

where $c \geq 2$ is an absolute constant (actually very close to 2).

What is a good lattice rule?

We showed that we can construct lattice rules such that the weighted star discrepancy is $O(n^{-1+\delta})$ for any $\delta > 0$. Such a bound is considered optimal.

Under certain conditions on the weights, the involved constant is independent of the dimension - this ensures **strong tractability**, hence no "curse of dimensionality".

Construction schemes

The total number of generating vectors for rank-1 lattice rules is $\varphi(n)^d$ so an exhaustive search among all possibilities is not practical. Thus there is a need to find reliable algorithms.

Construction schemes

A popular algorithm is the so-called "component-by-component" (CBC) construction. This is a **greedy**-type algorithm of a remarkable simplicity.

The central idea is, as the name suggests, finding the vector $\mathbf{z}$ a component at a time. So we set $z_1 = 1$ and find z_2. Once we have z_2, we fix it and then find z_3 etc.

A more difficult task is to show that the component-by-component construction will yield a good $\mathbf{z}$!

Component-by-component (CBC) algorithm

Let $z_1 := 1$.
For $m = 2, 3, \ldots, d$*:*
  find $z_m \in \mathcal{Z}_n$ *such that* $e_{n,m}(z_1, \ldots, z_m)$ *is minimised.*

A mathematical proof that this will produce indeed a good generating vector might be tedious, but is essential. In general terms, the proof is by induction over the dimension and consists of showing that it produces a generating vector that is at least as good as the average.

Fast CBC algorithm

As showed by Nuyens and Cools, a fast CBC construction can be used here to speed up the CBC algorithm by doing a fast matrix-vector multiplication in $O(n \log n)$ time instead of the usual $O(n^2)$. At a glance, the results can be summarised as follows.

- For general weights, we have a total cost of $O(n \log(n) d 2^d)$.
- For product weights, the total cost is $O(nd \log(n))$.
- For other particular classes of general weights, the total cost can also be $O(nd \log(n))$.

In each case, we have additional storage cost of at most $O(nd)$.

Other construction schemes

Korobov lattice rules - the generating vector is given by

$$\mathbf{z} := (1, a, \ldots, a^{d-1}) \pmod{n},$$

where $\gcd(a, n) = 1$.

Randomised CBC construction (at each step only a small number of random chosen possibilities are tested and the best one is chosen). Gives surprisingly good results!!

General weights and non-prime number of points

One can also proof that obtaining a lattice rule that is good with respect to the weighted star discrepancy, will also be good with respect to other figures of merit (such as the worst-case error in weighted Korobov spaces).

We obtain lattice rules whose weighted star discrepancy converges as $O(n^{-1+\delta})$ for any $\delta > 0$. We also established sufficient conditions of strong tractability (i.e. the constant involved is independent of the dimension).

Strong tractability

We established that if the weights are chosen such that

$$\lim_{d\to\infty} \sup_{n\geq n_0} n^{-\delta} \sum_{\mathfrak{u}\subseteq\mathcal{D}} \gamma_{\mathfrak{u}} (c \ln n)^{|\mathfrak{u}|} < \infty,$$

for any $\delta > 0$, then the bound $O(n^{-1+\delta})$ on the weighted star discrepancy is independent of the dimension.

We also proved that if the weights are product and satisfy the summability condition $\sum_{j=1}^{\infty} \gamma_j < \infty$, then our condition of strong tractability will hold as well. Hence, our conditions are not stronger than the known ones for product weights.

Strong tractability

We established that if the weights are chosen such that

$$\lim_{d\to\infty} \sup_{n\geq n_0} n^{-\delta} \sum_{\mathfrak{u}\subseteq\mathcal{D}} \gamma_{\mathfrak{u}}(c\ln n)^{|\mathfrak{u}|} < \infty,$$

for any $\delta > 0$, then the bound $O(n^{-1+\delta})$ on the weighted star discrepancy is independent of the dimension.

If the weights are finite-order ($\gamma_{\mathfrak{u}} = 0$ for any $\mathfrak{u}$ with $|\mathfrak{u}| \geq q$ with a fixed q) and satisfy the summability condition $\sum_{|\mathfrak{u}|<\infty} \gamma_{\mathfrak{u}} < \infty$, then our condition of strong tractability will hold as well.

Strong tractability

We established that if the weights are chosen such that

$$\lim_{d\to\infty} \sup_{n\geq n_0} n^{-\delta} \sum_{\mathfrak{u}\subseteq\mathcal{D}} \gamma_{\mathfrak{u}} (c \ln n)^{|\mathfrak{u}|} < \infty,$$

for any $\delta > 0$, then the bound $O(n^{-1+\delta})$ on the weighted star discrepancy is independent of the dimension.

We also would like to have a better characterisation of general weights (for instance order-dependent weights), but this is still an open problem!

Why is the non-prime case more difficult?

In order to get the results for the mean and for the CBC construction, we use an averaging argument that involves the quantity

$$T_n(k) := \frac{1}{\varphi(n)} \sum_{z \in \mathcal{Z}_n} \sideset{}{'}\sum_{-n/2 < h \leq n/2} \frac{e^{2\pi i h k z / n}}{|h|},$$

for $1 \leq k \leq n-1$.
A number theory problem: Find a closed form formula for $T_n(k)$.

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for $1 \leq k \leq n-1$.
If n is prime, then

$$T_n(k) = -\frac{S_n}{n-1},$$

for every k, where $S_n := \sum'_{-n/2<h\leq n/2} 1/|h|$. It is known that $S_n \leq 2 \ln n$.

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for $1 \le k \le n-1$.
When n is non-prime, then the best known result is due to Niederreiter:

$$T_n(k) = -\frac{2 \ln p}{p^{\alpha_k}(p-1)} + O\left(\frac{1}{\varphi(n)}\right),$$

with an absolute implied constant. Above, p is a prime that divides both k and n. This is still not enough for our analysis!

Why is the non-prime case more difficult?

We proved that

$$\sum_{k=1}^{n-1} |T_n(k)| \leq c \ln n,$$

with the constant $c \geq 2$.

This result was crucial in developing the underlying theory in the non-prime case.

On the real value of the star discrepancy

The real value of the weighted star discrepancy can be quite far away from its bounds.

The bounds will give us more information on how good a lattice rule is and less on what is the real order of magnitude of the error.

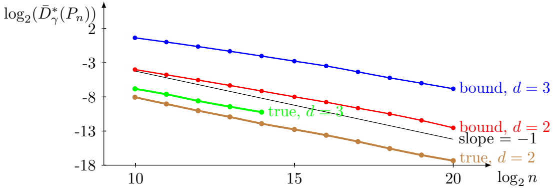

Figure 1: The best bound on the weighted star discrepancy of lattice rules obtained with the CBC construction as a function of n, in a log-log scale, in $d = 2, 3$ dimensions, when $\gamma_j = 1$ for all j. We also have the true weighted star discrepancy $D^*_{n,\gamma}(\mathbf{z})$ for the cases where computation could be done reasonably fast (for $d = 2$ and for $d = 3$ with small n).

Conclusions

1. Among other types of figures of merit, the weighted star discrepancy requires less smoothness assumptions for the integrand.
2. Allows to obtain lattice rules that are also good with respect to other figures of merit.
3. We established sufficient conditions on tractability .
4. One disadvantage is that the computed bounds are considerably larger than the real values.

Conclusions

1. Better algorithm for computing the discrepancy would be useful.
2. Perhaps better bounds are also possible.
3. More to be said about the weighted star discrepancy of other QMC point sets?

Thank you !