

Error Estimation for Quasi-Monte Carlo Methods

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Abstract

Keywords:

1. Bases and Node Sets

1.1. Group-Like Structures

Consider the half open d -dimensional unit cube, $\mathcal{X} := [0, 1)^d$, on which the functions of interest are to be defined. Suppose that there exists a commutative unital structure on \mathcal{X} , i.e., there exists a commutative addition operation $\oplus : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{X}$ with identity element $\mathbf{0}$ (the zero vector):

$$\mathbf{x} \oplus \mathbf{t} = \mathbf{t} \oplus \mathbf{x}, \quad \mathbf{x} \oplus \mathbf{0} = \mathbf{x} \quad \forall \mathbf{x}, \mathbf{t} \in \mathcal{X}.$$

Every $\mathbf{x} \in \mathcal{X}$ is assumed to have a unique additive inverse, denoted $\ominus \mathbf{x}$, and $\mathbf{x} \ominus \mathbf{t}$ means $\mathbf{x} \oplus (\ominus \mathbf{t})$. Thus, $\mathbf{x} \ominus \mathbf{x} = \mathbf{0}$. Associativity is not assumed, and so there may exist $\mathbf{t} \in \mathcal{X}$, $\mathbf{t} \neq \ominus \mathbf{x}$, such that $\mathbf{x} \oplus \mathbf{t} = \mathbf{0}$. This means that \mathcal{X} might not be a group.

However, it is assumed that for some subsets of \mathcal{X} , denoted $\tilde{\mathcal{X}}$, which are closed under \oplus and for which associativity also holds:

$$\mathbf{x} \oplus (\mathbf{t} \oplus \mathbf{u}) = (\mathbf{x} \oplus \mathbf{t}) \oplus \mathbf{u} \quad \forall \mathbf{x}, \mathbf{t}, \mathbf{u} \in \tilde{\mathcal{X}}. \quad (1)$$

As a consequence, such subsets, $\tilde{\mathcal{X}}$, are commutative groups.

Let \mathbb{K} denote some subset of the d -dimensional vector of integers that contains $\mathbf{0}$. Important examples are the set of integer vectors, \mathbb{Z}^d , and the set of non-negative integer vectors, \mathbb{N}_0^d . The set \mathbb{K} is used to index the series expressions for the functions to be integrated. Suppose also that there exists an Abelian group structure on \mathbb{K} , with the additive operation \oplus . Moreover, assume that there exists an operation $\otimes : \mathbb{K} \times \mathcal{X} \rightarrow [0, 1)$ that returns zero if either argument is zero and also has a distributive property:

$$\mathbf{k} \otimes \mathbf{0} = \mathbf{0} \otimes \mathbf{x} = 0 \quad \forall \mathbf{k} \in \mathbb{K}, \mathbf{x} \in \mathcal{X}, \quad (2a)$$

$$\mathbf{k} \otimes (\mathbf{x} \oplus \mathbf{t}) = (\mathbf{k} \otimes \mathbf{x}) + (\mathbf{k} \otimes \mathbf{t}) \pmod{1} \quad \forall \mathbf{k} \in \mathbb{K}, \mathbf{x} \in \mathcal{X}, \mathbf{t} \in \tilde{\mathcal{X}}, \quad (2b)$$

$$(\mathbf{k} \oplus \mathbf{l}) \otimes \mathbf{x} = (\mathbf{k} \otimes \mathbf{x}) + (\mathbf{l} \otimes \mathbf{x}) \pmod{1} \quad \forall \mathbf{k}, \mathbf{l} \in \mathbb{K}, \mathbf{x} \in \mathcal{X}. \quad (2c)$$

1.2. Examples of Group-Like Structures

The general notation introduced in the previous subsection and continued in the subsections below is intended to include the algebra behind both *integration lattices* and *digital nets*. This subsection defines these two special kinds of operators \oplus , \ominus and \otimes .

Integration lattices are sets that are closed under addition and subtraction modulo one. In this setting $\mathbb{K} = \mathbb{Z}^d$, and

$$\begin{aligned} \mathbf{x} \oplus \mathbf{t} &= \mathbf{x} + \mathbf{t} \pmod{1}, & \ominus \mathbf{x} &= -\mathbf{x} \pmod{1} & \forall \mathbf{x}, \mathbf{t} \in \mathcal{X}, \\ \mathbf{k} \oplus \mathbf{l} &= \mathbf{k} + \mathbf{l}, & \ominus \mathbf{k} &= -\mathbf{k} & \forall \mathbf{k}, \mathbf{l} \in \mathbb{K}, \\ \mathbf{k} \otimes \mathbf{x} &= \mathbf{k}^T \mathbf{x} \pmod{1} & \forall \mathbf{x} \in \mathcal{X}, \mathbf{k} \in \mathbb{K}. \end{aligned}$$

All the properties of the previous section can be shown to hold. Specifically, associativity, (1), and the distributive property, (2), hold for $\tilde{\mathcal{X}} = \mathcal{X} = [0, 1)^d$, so \mathcal{X} is a group.

The digital net setting deals with b -ary expansions of \mathcal{X} , where b is prime, and $\mathbb{K} = \mathbb{N}_0^d$. Let $\mathbf{x} = (x_1, \dots, x_d)$, and let $x_j = {}_b0.x_{j1}x_{j2}\dots$ be the proper b -ary expansion (no infinite trail of $b-1$ s) of $x_j \in [0, 1)$. Furthermore, let $\mathbf{k} = (k_1, \dots, k_d)$, and let $k_j = (\dots k_{j2}k_{j1})_b$ be the b -ary expansion of $k_j \in \mathbb{N}_0$. Specifically

$$\begin{aligned} \mathbf{x} &= \left(\sum_{\ell=1}^{\infty} x_{j\ell} b^{-\ell} \right)_{j=1}^d, & \ominus \mathbf{x} &= \left(\sum_{\ell=1}^{\infty} [-x_{j\ell} \bmod b] b^{-\ell} \right)_{j=1}^d & \forall \mathbf{x} \in \mathcal{X} \\ \mathbf{x} \oplus \mathbf{t} &= \left(\sum_{\ell=1}^{\infty} [x_{j\ell} + t_{j\ell} \bmod b] b^{-\ell} \right)_{j=1}^d & \forall \mathbf{x}, \mathbf{t} \in \mathcal{X}, \\ \mathbf{k} &= \left(\sum_{\ell=0}^{\infty} k_{j\ell} b^{\ell} \right)_{j=1}^d, & \ominus \mathbf{k} &= \left(\sum_{\ell=0}^{\infty} [-k_{j\ell} \bmod b] b^{\ell} \right)_{j=1}^d & \forall \mathbf{k} \in \mathbb{K}, \\ \mathbf{k} \oplus \mathbf{l} &= \left(\sum_{\ell=0}^{\infty} [k_{j\ell} + l_{j\ell} \bmod b] b^{\ell} \right)_{j=1}^d & \forall \mathbf{k}, \mathbf{l} \in \mathbb{K}, \\ \mathbf{k} \otimes \mathbf{x} &= \left(\left[\frac{1}{b} \sum_{\ell=0}^{\infty} k_{j\ell} x_{j,\ell+1} \right] \bmod 1 \right)_{j=1}^d & \forall \mathbf{x} \in \mathcal{X}, \mathbf{k} \in \mathbb{K}. \end{aligned}$$

What is $\tilde{\mathcal{X}}$?

1.3. Fourier Series

The integrands are assumed to belong to some subset of $\mathcal{L}_2(\mathcal{X})$, the space of square integrable functions. The \mathcal{L}_2 inner product is defined as

$$\langle f, g \rangle_2 = \int_{\mathcal{X}} f(\mathbf{x}) \overline{g(\mathbf{x})} d\mathbf{x}.$$

Let $\{\varphi(\cdot, \mathbf{k}) \in \mathcal{L}_2(\mathcal{X}) : \mathbf{k} \in \mathbb{K}\}$ be some complete orthonormal *basis* for $\mathcal{L}_2(\mathcal{X})$. In particular, let

$$\varphi(\mathbf{x}, \mathbf{k}) = e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{x}}, \quad \mathbf{k} \in \mathbb{K}, \mathbf{x} \in \mathcal{X}.$$

Then any function in \mathcal{L}_2 may be written in series form as

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{K}} \hat{f}(\mathbf{k}) \varphi(\mathbf{x}, \mathbf{k}), \quad \text{where } \hat{f}(\mathbf{k}) = \langle f, \varphi(\cdot, \mathbf{k}) \rangle_2, \quad (3)$$

and the inner product of two functions in \mathcal{L}_2 is the ℓ_2 inner product of their series coefficients:

$$\langle f, g \rangle_2 = \sum_{\mathbf{k} \in \mathbb{K}} \hat{f}(\mathbf{k}) \overline{\hat{g}(\mathbf{k})} =: \left\langle (\hat{f}(\mathbf{k}))_{\mathbf{k} \in \mathbb{K}}, (\hat{g}(\mathbf{k}))_{\mathbf{k} \in \mathbb{K}} \right\rangle_2.$$

1.4. Node Sets and Their Dual Sets

Now suppose that \mathcal{P} is any finite subgroup of $\tilde{\mathcal{X}}$ with cardinality $|\mathcal{P}|$. This will be called a *node set*. It then follows that for all $\mathbf{k} \in \mathbb{K}$ and $\mathbf{t} \in \mathcal{P}$,

$$\begin{aligned} 0 &= \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} [\varphi(\mathbf{x}, \mathbf{k}) - \varphi(\mathbf{x} \oplus \mathbf{t}, \mathbf{k})] = \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} [e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{x}} - e^{2\pi\sqrt{-1}\mathbf{k}\otimes(\mathbf{x}\oplus\mathbf{t})}] \\ &= \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} [e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{x}} - e^{2\pi\sqrt{-1}\{(\mathbf{k}\otimes\mathbf{x})+(\mathbf{k}\otimes\mathbf{t})\}}] \quad \text{by (2)} \\ &= [1 - e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{t}}] \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{x}}. \end{aligned} \quad (4)$$

Define the *dual set* corresponding to \mathcal{P} as

$$\mathcal{P}^\perp = \{\mathbf{k} \in \mathbb{K} : \mathbf{k} \otimes \mathbf{x} = 0 \ \forall \mathbf{x} \in \mathcal{P}\}.$$

The distributive property, (2), implies that dual set is a subgroup of \mathbb{K} . By the equality (4) above it follows that the average of a basis function, $\varphi(\cdot, \mathbf{k})$, over the points in a node set is either one or zero, depending on whether \mathbf{k} is in the dual set or not.

$$\frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{x}} = \mathbb{1}_{\mathcal{P}^\perp}(\mathbf{k}) = \begin{cases} 1, & \mathbf{k} \in \mathcal{P}^\perp \\ 0, & \mathbf{k} \in \mathbb{K} \setminus \mathcal{P}^\perp. \end{cases}$$

A *shifted* node set is constructed by adding the same point $\mathbf{\Delta} \in \mathcal{X}$ to each element in the node set:

$$\mathcal{P}_\mathbf{\Delta} = \{\mathbf{x} + \mathbf{\Delta} : \mathbf{x} \in \mathcal{P}\}.$$

$$\begin{aligned} \frac{1}{|\mathcal{P}_\mathbf{\Delta}|} \sum_{\mathbf{x} \in \mathcal{P}_\mathbf{\Delta}} e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{x}} &= \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} e^{2\pi\sqrt{-1}\mathbf{k}\otimes(\mathbf{x}\oplus\mathbf{\Delta})} = \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} e^{2\pi\sqrt{-1}[(\mathbf{k}\otimes\mathbf{x})+(\mathbf{k}\otimes\mathbf{\Delta})]} \\ &= e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{\Delta}} \mathbb{1}_{\mathcal{P}^\perp}(\mathbf{k}) = \begin{cases} e^{2\pi\sqrt{-1}\mathbf{k}\otimes\mathbf{\Delta}}, & \mathbf{k} \in \mathcal{P}^\perp \\ 0, & \mathbf{k} \in \mathbb{K} \setminus \mathcal{P}^\perp. \end{cases} \end{aligned}$$

1.5. Discrete Transforms

Define the discrete transform of a function, f , over the shifted node set \mathcal{P}_Δ as

$$\begin{aligned}
\tilde{f}(\mathbf{k}) &:= \frac{1}{|\mathcal{P}_\Delta|} \sum_{\mathbf{x} \in \mathcal{P}_\Delta} e^{-2\pi\sqrt{-1}\mathbf{k} \otimes \mathbf{x}} f(\mathbf{x}) \\
&= \frac{1}{|\mathcal{P}_\Delta|} \sum_{\mathbf{x} \in \mathcal{P}_\Delta} \left[e^{-2\pi\sqrt{-1}\mathbf{k} \otimes \mathbf{x}} \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\mathbf{l} \otimes \mathbf{x}} \right] \\
&= \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) \frac{1}{|\mathcal{P}_\Delta|} \sum_{\mathbf{x} \in \mathcal{P}_\Delta} e^{2\pi\sqrt{-1}(\mathbf{l} \ominus \mathbf{k}) \otimes \mathbf{x}} \\
&= \sum_{\substack{\mathbf{l} \in \mathbb{K} \\ \mathbf{l} \ominus \mathbf{k} \in \mathcal{P}^\perp}} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}(\mathbf{l} \ominus \mathbf{k}) \otimes \Delta} \\
&= \sum_{\mathbf{m} \in \mathcal{P}^\perp} \hat{f}(\mathbf{k} \oplus \mathbf{m}) e^{2\pi\sqrt{-1}\mathbf{m} \otimes \Delta}, \\
&= \hat{f}(\mathbf{k}) + \sum_{\mathbf{m} \in \mathcal{P}^\perp \setminus \mathbf{0}} \hat{f}(\mathbf{k} \oplus \mathbf{m}) e^{2\pi\sqrt{-1}\mathbf{m} \otimes \Delta}, \quad \forall \mathbf{k} \in \mathbb{K}.
\end{aligned} \tag{5}$$

It is seen here that the discrete transform $\tilde{f}(\mathbf{k})$ is equal to the integral transform $\hat{f}(\mathbf{k})$, defined in (3), plus the *aliasing* terms corresponding to $\hat{f}(\mathbf{l})$ where \mathbf{l} and \mathbf{k} differ (in the \ominus sense) by a nonzero element of the dual set.

Notice that the dual nets can be used to form cosets of wavenumbers. Let

$$\mathcal{P}_\mathbf{k}^\perp = \{\mathbf{l} \in \mathbb{K} : \mathbf{l} \ominus \mathbf{k} \in \mathcal{P}^\perp\}.$$

This means that $\mathcal{P}_\mathbf{0}^\perp = \mathcal{P}^\perp$. There are $|\mathcal{P}|$ distinct cosets. Then (6) above implies that

$$\tilde{f}(\mathbf{k}) = \sum_{\mathbf{l} \in \mathcal{P}_\mathbf{k}^\perp} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}(\mathbf{l} \ominus \mathbf{k}) \otimes \Delta}. \tag{7}$$

Now consider the situation where there is a sequence of nested sets,

$$\mathcal{P}_0 = \{\mathbf{0}\} \subset \mathcal{P}_1 \subset \mathcal{P}_2 \subset \dots, \quad |\mathcal{P}_r| = b^r$$

Furthermore, assume that each set equals the previous plus multiples of one element:

$$\mathcal{P}_r = \{\mathbf{x} \oplus \mathbf{t} : \mathbf{x} \in \mathcal{P}_{r-1}, \mathbf{t} \in \{\mathbf{0}, \mathbf{z}_r, \mathbf{z}_r \oplus \mathbf{z}_r, \dots\}\}, \quad r = 1, 2, \dots,$$

where $\mathbf{z}_1, \mathbf{z}_2, \dots \in \tilde{\mathcal{X}}$ is some fixed sequence. According to this definition of nested sets, the dual sets are nested in the opposite direction,

$$\mathcal{P}_0^\perp = \mathbb{K} \supset \mathcal{P}_1^\perp \supset \mathcal{P}_2^\perp \supset \dots.$$

Now we are going to map the non-negative numbers into the space of all wavenumbers using the dual sets. For every $\kappa \in \mathbb{N}_0$, we assign a wavenumber $\mathbf{k}(\kappa) \in \mathbb{K}$ iteratively as follows.

- Let $\mathbf{k}(0) = \mathbf{0}$.
- For any $\kappa = \kappa_0 + \kappa_1 b + \kappa_2 b^2 + \cdots + \kappa_{r-1} b^{r-1}$ and any $\kappa' = \kappa_0 + \kappa_1 b + \kappa_2 b^2 + \cdots + \kappa_{r-1} b^{r-1} + \kappa'_r b^r + \cdots + \kappa'_{r'} b^{r'+1}$, where κ_j and κ'_j are integers between 0 and $b-1$, assign $\mathbf{k}(\kappa)$ and $\mathbf{k}(\kappa')$ such that $\mathcal{P}_{r, \mathbf{k}(\kappa)}^\perp$ and $\mathcal{P}_{r, \mathbf{k}(\kappa')}^\perp$ the same equivalence class.

Introducing the shorthand notation such $\hat{f}_\kappa = \hat{f}(\mathbf{k}(\kappa))$, and such that $\tilde{f}_{\kappa, r}$ corresponds to the discrete transform $\tilde{f}(\mathbf{k}(\kappa))$ defined in (5) based on the shifted nodeset $\mathcal{P}_{r, \Delta}$. Likewise, $\mathcal{P}_{\kappa, r}^\perp$ denote the coset $\mathcal{P}_{\mathbf{k}(\kappa), r}^\perp$ for $\kappa = 0, \dots, b^r - 1$. According to (7), it follows that

$$\begin{aligned}
\tilde{f}_{\kappa, r} &= \sum_{\mathbf{l} \in \mathcal{P}_{\kappa, r}^\perp} \hat{f}(\mathbf{l}) e^{2\pi \sqrt{-1}(\mathbf{l} \ominus \mathbf{k}(\kappa)) \otimes \Delta} \\
&= \sum_{\lambda=0}^{\infty} \hat{f}_{\kappa + \lambda b^r} e^{2\pi \sqrt{-1}(\mathbf{l}(\kappa + \lambda b^r) \ominus \mathbf{k}(\kappa)) \otimes \Delta} \\
&= \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa + \lambda b^r} e^{2\pi \sqrt{-1}(\mathbf{l}(\kappa + \lambda b^r) \ominus \mathbf{k}(\kappa)) \otimes \Delta}.
\end{aligned} \tag{8}$$

We want to use $\tilde{f}_{\kappa, r}$ to estimate \hat{f}_κ if r is larger enough than $\lfloor \log_b(\kappa) \rfloor$.

Consider the following sums

$$S(r) = \sum_{\kappa=b^r}^{b^{r+1}-1} \left| \hat{f}_\kappa \right|, \quad r \in \mathbb{N}_0, \tag{9}$$

$$\tilde{S}(\kappa, r_1, r_2) = \sum_{\lambda=b^{r_2}}^{b^{r_2+1}-1} \left| \hat{f}_{\kappa + \lambda b^{r_1}} \right|, \quad \kappa = 0, \dots, b^{r_1} - 1, \quad r_1, r_2 \in \mathbb{N}_0, \tag{10}$$

$$\hat{S}(r, r_1, r_2) = \sum_{\lambda=b^r}^{b^{r+1}-1} \tilde{S}(\kappa, r_1, r_2), \quad r = 0, \dots, r_1 - 1, \quad r_1, r_2 \in \mathbb{N}_0, \tag{11}$$

We make the critical assumption that these sums decay with increasing r_1 and r_2 , namely,

$$S(r, r_1, r_2) \leq s_1 s_2^{r_1 + r_2 - r} S(r, r_1, r_2), \quad r \geq r_{\min}, \tag{12}$$