# 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 unidal structure on $\mathcal{X}$, i.e., there exists a commutative addition operation $\oplus : \mathcal{X} \times \mathcal{X} \to \mathcal{X}$ with identity element $\mathbf{0}$ (the zero vector):

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

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

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

$$\boldsymbol{x} \oplus (\boldsymbol{t} \oplus \boldsymbol{u}) = (\boldsymbol{x} \oplus \boldsymbol{t}) \oplus \boldsymbol{u} \qquad \forall \boldsymbol{x}, \boldsymbol{t}, \boldsymbol{u} \in \widetilde{\mathcal{X}}. \tag{1}$$

As a consequence, such subsets, $\widetilde{\mathcal{X}}$, 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 $\otimes : \mathbb{K} \times \mathcal{X} \to [0,1)$ that returns zero if either argument is zero and also has a distributive property:

$$\boldsymbol{k} \otimes \mathbf{0} = \mathbf{0} \otimes \boldsymbol{x} = 0 \qquad \forall \boldsymbol{k} \in \mathbb{K}, \boldsymbol{x} \in \mathcal{X}, \tag{2a}$$

$$\boldsymbol{k} \otimes (\boldsymbol{x} \oplus \boldsymbol{t}) = (\boldsymbol{k} \otimes \boldsymbol{x}) + (\boldsymbol{k} \otimes \boldsymbol{t}) \pmod 1 \qquad \forall \boldsymbol{k} \in \mathbb{K}, \boldsymbol{x} \in \mathcal{X}, \boldsymbol{t} \in \widetilde{\mathcal{X}}, \tag{2b}$$

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

*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

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

All the properties of the previous section can be shown to hold. Specifically, associativity, (1), and the distributive property, (2), hold for $\widetilde{\mathcal{X}} = \mathcal{X} = [0,1)^d$, 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 $\boldsymbol{x} = (x_1, \ldots, x_d)$, and let $x_j = {}_b0.x_{j1}x_{j2}\cdots$ be the proper $b$-ary expansion (no infinite trail of $b-1$s) of $x_j \in [0,1)$. Furthermore, let $\boldsymbol{k} = (k_1, \ldots, k_d)$, and let $k_j = (\cdots k_{j2}k_{j1})_b$ be the $b$-ary expansion of $k_j \in \mathbb{N}_0$. Specifically

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

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

*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

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

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

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

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

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

and the inner product of two functions in $\mathcal{L}_2$ is the $\ell_2$ inner product of their series coefficients:

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

*1.4. Node Sets and Their Dual Sets*

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

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

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

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

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, $\varphi(\cdot,\boldsymbol{k})$, over the points in a node set is either one or zero, depending on whether $\boldsymbol{k}$ is in the dual set or not.

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

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

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

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

*1.5. Discrete Transforms*

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

$$\begin{aligned}
\tilde{f}(\boldsymbol{k}) &:= \frac{1}{|\mathcal{P}_{\boldsymbol{\Delta}}|} \sum_{\boldsymbol{x} \in \mathcal{P}_\Delta} \mathrm{e}^{-2\pi\sqrt{-1}\boldsymbol{k}\otimes\boldsymbol{x}} f(\boldsymbol{x}) && (5) \\
&= \frac{1}{|\mathcal{P}_{\boldsymbol{\Delta}}|} \sum_{\boldsymbol{x} \in \mathcal{P}_\Delta} \left[ \mathrm{e}^{-2\pi\sqrt{-1}\boldsymbol{k}\otimes\boldsymbol{x}} \sum_{\boldsymbol{l} \in \mathbb{K}} \hat{f}(\boldsymbol{l}) \mathrm{e}^{2\pi\sqrt{-1}\boldsymbol{l}\otimes\boldsymbol{x}} \right] \\
&= \sum_{\boldsymbol{l}s \in \mathbb{K}} \hat{f}(\boldsymbol{l}) \frac{1}{|\mathcal{P}_{\boldsymbol{\Delta}}|} \sum_{\boldsymbol{x} \in \mathcal{P}_{\boldsymbol{\Delta}}} \mathrm{e}^{2\pi\sqrt{-1}(\boldsymbol{l}\ominus\boldsymbol{k})\otimes\boldsymbol{x}} \\
&= \sum_{\substack{\boldsymbol{l} \in \mathbb{K} \\ \boldsymbol{l}\ominus\boldsymbol{k} \in \mathcal{P}^\perp}} \hat{f}(\boldsymbol{l}) \mathrm{e}^{2\pi\sqrt{-1}(\boldsymbol{l}\ominus\boldsymbol{k})\otimes\boldsymbol{\Delta}} \\
&= \sum_{\boldsymbol{m} \in \mathcal{P}^\perp} \hat{f}(\boldsymbol{k} \oplus \boldsymbol{m}) \mathrm{e}^{2\pi\sqrt{-1}\boldsymbol{m}\otimes\boldsymbol{\Delta}}, \\
&= \hat{f}(\boldsymbol{k}) + \sum_{\boldsymbol{m} \in \mathcal{P}^\perp \setminus \boldsymbol{0}} \hat{f}(\boldsymbol{k} \oplus \boldsymbol{m}) \mathrm{e}^{2\pi\sqrt{-1}\boldsymbol{m}\otimes\boldsymbol{\Delta}}, \qquad \forall \boldsymbol{k} \in \mathbb{K}. && (6)
\end{aligned}$$

It is seen here that the discrete transform $\tilde{f}(\boldsymbol{k})$ is equal to the integral transform $\hat{f}(\boldsymbol{k})$, defined in (3), plus the *aliasing* terms corresponding to $\hat{f}(\boldsymbol{l})$ where $\boldsymbol{l}$ and $\boldsymbol{k}$ 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

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

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

$$\tilde{f}(\boldsymbol{k}) = \sum_{\boldsymbol{l} \in \mathcal{P}^\perp_{\boldsymbol{k}}} \hat{f}(\boldsymbol{l}) \mathrm{e}^{2\pi\sqrt{-1}(\boldsymbol{l}\ominus\boldsymbol{k})\otimes\boldsymbol{\Delta}}. \qquad (7)$$

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

$$\mathcal{P}_0 = \{\boldsymbol{0}\} \subset \mathcal{P}_1 \subset \mathcal{P}_2 \subset \cdots, \qquad |\mathcal{P}_r| = b^r$$

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

$$\mathcal{P}_r = \{\boldsymbol{x} \oplus \boldsymbol{t} : \boldsymbol{x} \in \mathcal{P}_{r-1},\ \boldsymbol{t} \in \{\boldsymbol{0}, \boldsymbol{z}_r, \boldsymbol{z}_r \oplus \boldsymbol{z}_r, \ldots\}\}, \qquad r = 1, 2, \ldots,$$

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

$$\mathcal{P}^\perp_0 = \mathbb{K} \supset \mathcal{P}^\perp_1 \supset \mathcal{P}^\perp_2 \supset \cdots.$$

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 $\boldsymbol{k}(\kappa) \in \mathbb{K}$ iteratively as follows.

- Let $\boldsymbol{k}(0) = \boldsymbol{0}$.
- 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 $\kappa_j$ and $\kappa'_j$ are integers between 0 and $b-1$, assign $\boldsymbol{k}(\kappa)$ and $\boldsymbol{k}(\kappa')$ such that $\mathcal{P}^{\perp}_{r,\boldsymbol{k}(\kappa)}$ and $\mathcal{P}^{\perp}_{r,\boldsymbol{k}(\kappa')}$ the same equivalence class.

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

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

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

Consider the following sums

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

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

$$
\widehat{S}(r, r_1, r_2) = \sum_{\lambda=b^r}^{b^{r+1}-1} \widetilde{S}(\kappa, r_1, r_2), \qquad r = 0, \ldots, r_1 - 1,\ r_1, r_2 \in \mathbb{N}_0, \tag{11}
$$

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

$$
S(r, r_1, r_2) \le s_1 s_2^{r_1+r_2-r} S(r, r_1, r_2), \qquad r \ge r_{\min}, \tag{12}
$$