

Error Estimation for Quasi-Monte Carlo Methods

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Abstract

Keywords:

1. Bases and Node Sets

1.1. Group-Like Structure

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

$$\mathbf{x} \oplus \mathbf{t} = \mathbf{x} + \mathbf{t} \pmod{1}, \quad \ominus \mathbf{x} = -\mathbf{x} \pmod{1} \quad \forall \mathbf{x}, \mathbf{t} \in \mathcal{X}.$$

Under this operation, (\mathcal{X}, \oplus) is a commutative group.

Let $\mathbb{K} := \mathbb{Z}^d$. This set is used to index the series expressions for the functions to be integrated. $(\mathbb{K}, +)$ is also an Abelian group, with the regular additive operation. Moreover, define the operation $\langle \cdot, \cdot \rangle : \mathbb{K} \times \mathcal{X} \rightarrow [0, 1)$ that has a distributive property under \oplus and $+$:

$$\langle \mathbf{k}, \mathbf{x} \rangle = \mathbf{k}^T \mathbf{x} \pmod{1} \quad \forall \mathbf{x} \in \mathcal{X}, \mathbf{k} \in \mathbb{K} \quad (1a)$$

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

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

This is the algebra behind *integration lattices*.

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

$$\mathbf{x} \oplus \mathbf{t} = \mathbf{x} + \mathbf{t} \pmod{1}, \quad \ominus \mathbf{x} = -\mathbf{x} \pmod{1} \quad \forall \mathbf{x}, \mathbf{t} \in \mathcal{X},$$

$$\mathbf{k} \oplus \mathbf{l} = \mathbf{k} + \mathbf{l}, \quad \ominus \mathbf{k} = -\mathbf{k} \quad \forall \mathbf{k}, \mathbf{l} \in \mathbb{K},$$

$$\mathbf{k} \otimes \mathbf{x} = \mathbf{k}^T \mathbf{x} \pmod{1} \quad \forall \mathbf{x} \in \mathcal{X}, \mathbf{k} \in \mathbb{K}.$$

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

1.2. 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

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

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

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{K}} \hat{f}(\mathbf{k}) \varphi(\mathbf{x}, \mathbf{k}), \quad \text{where } \hat{f}(\mathbf{k}) = \langle f, \varphi(\cdot, \mathbf{k}) \rangle_2, \quad (2)$$

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

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

1.3. Node Sets and Their Dual Sets

Now suppose that \mathcal{P} is any finite subgroup of \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 $\mathbf{t} \in \mathcal{P}$,

$$\begin{aligned} 0 &= \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} [\varphi(\mathbf{x}, \mathbf{k}) - \varphi(\mathbf{x} \oplus \mathbf{t}, \mathbf{k})] = \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} [e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle} - e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \oplus \mathbf{t} \rangle}] \\ &= \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} [e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle} - e^{2\pi\sqrt{-1}\{\langle \mathbf{k}, \mathbf{x} \rangle + \langle \mathbf{k}, \mathbf{t} \rangle\}}] \quad \text{by (1)} \\ &= [1 - e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t} \rangle}] \frac{1}{|\mathcal{P}|} \sum_{\mathbf{x} \in \mathcal{P}} e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle}. \end{aligned} \quad (3)$$

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

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

The distributive property, (1), implies that dual set is a subgroup of \mathbb{K} . By the equality (3) 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:

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

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

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

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

1.4. Discrete Transforms

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

$$\begin{aligned} \tilde{f}(\mathbf{k}) &:= \frac{1}{|\mathcal{P}_\Delta|} \sum_{\mathbf{x} \in \mathcal{P}_\Delta} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle} f(\mathbf{x}) \tag{4} \\ &= \frac{1}{|\mathcal{P}_\Delta|} \sum_{\mathbf{x} \in \mathcal{P}_\Delta} \left[e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle} \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l}, \mathbf{x} \rangle} \right] \\ &= \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) \frac{1}{|\mathcal{P}_\Delta|} \sum_{\mathbf{x} \in \mathcal{P}_\Delta} e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \mathbf{x} \rangle} \\ &= \sum_{\substack{\mathbf{l} \in \mathbb{K} \\ \mathbf{l} \ominus \mathbf{k} \in \mathcal{P}^\perp}} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \Delta \rangle} \\ &= \sum_{\mathbf{m} \in \mathcal{P}^\perp} \hat{f}(\mathbf{k} \oplus \mathbf{m}) e^{2\pi\sqrt{-1}\langle \mathbf{m}, \Delta \rangle}, \\ &= \hat{f}(\mathbf{k}) + \sum_{\mathbf{m} \in \mathcal{P}^\perp \setminus \mathbf{0}} \hat{f}(\mathbf{k} \oplus \mathbf{m}) e^{2\pi\sqrt{-1}\langle \mathbf{m}, \Delta \rangle}, \quad \forall \mathbf{k} \in \mathbb{K}. \tag{5} \end{aligned}$$

It is seen here that the discrete transform $\tilde{f}(\mathbf{k})$ is equal to the integral transform $\hat{f}(\mathbf{k})$, defined in (2), 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

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

This means that $\mathcal{P}_\mathbf{0}^\perp = \mathcal{P}^\perp$. Then (5) above implies that

$$\tilde{f}(\mathbf{k}) = \sum_{\mathbf{l} \in \mathcal{P}_\mathbf{k}^\perp} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \Delta \rangle}. \tag{6}$$

Note that there are $|\mathcal{P}|$ distinct cosets.

1.5. Nested Node Sets and Their Corresponding Nested Dual Sets

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

$$\mathcal{P}_0 = \{\mathbf{0}\} \subset \mathcal{P}_1 \subset \mathcal{P}_2 \subset \cdots, \quad |\mathcal{P}_s| = 2^s$$

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

$$\mathcal{P}_s = \{\mathbf{x} \oplus \mathbf{t} : \mathbf{x} \in \mathcal{P}_{s-1}, \mathbf{t} \in \{\mathbf{0}, \mathbf{z}_s, \mathbf{z}_s \oplus \mathbf{z}_s, \dots, \underbrace{\mathbf{z}_s \oplus \cdots \oplus \mathbf{z}_s}_{b-1 \text{ times}}\}\}, \quad s \in \mathbb{N}$$

where $\mathbf{z}_1, \mathbf{z}_2, \dots \in \mathcal{X}$ is some fixed sequence. See that $\{\mathbf{0}, \mathbf{z}_s, \mathbf{z}_s \oplus \mathbf{z}_s, \dots, \underbrace{\mathbf{z}_s \oplus \cdots \oplus \mathbf{z}_s}_{b-1 \text{ times}}\}$

is a subgroup of \mathcal{X} , defined as \mathcal{Z}_s . According to this definition of nested sets, the dual sets are nested in the opposite direction,

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

Furthermore, the equivalence classes also obey this nesting:

$$\mathcal{P}_{s,\mathbf{k}}^\perp = \{\mathbf{l} \in \mathbb{K} : \mathbf{l} \ominus \mathbf{k} \in \mathcal{P}_s^\perp\}, \quad \mathcal{P}_{0,\mathbf{k}}^\perp = \mathbb{K} \supset \mathcal{P}_{1,\mathbf{k}}^\perp \supset \mathcal{P}_{2,\mathbf{k}}^\perp \supset \cdots \quad \forall \mathbf{k} \in \mathbb{K}.$$

The discrete transforms of for nested sets can be constructed iteratively. Suppose that the points in these nested sets are ordered such that $\mathcal{P}_{s,\Delta} = \{\mathbf{x}_0, \dots, \mathbf{x}_{2^s-1}\}$ for some infinite sequence, $\{\mathbf{x}_i\}_{i=0}^\infty$. Furthermore, suppose that

$$\mathbf{x}_{i+j2^s} = \mathbf{x}_i \oplus \underbrace{\mathbf{z}_s \oplus \cdots \oplus \mathbf{z}_s}_{j \text{ times}}, \quad i = 0, \dots, 2^{s-1} - 1, \quad j = 0, \dots, b-1.$$

Nested rank-1 integration lattices are constructed in terms of the radical inverse function, as in []:

$$\mathbf{x}_i = \mathbf{h}\phi_b(i) \pmod{1}, \quad (7a)$$

where \mathbf{h} is a d -dimensional generating vector of ??? integers

$$\phi_b(i) = i_0 2^{-1} + i_1 2^{-2} + \cdots, \quad i = i_0 + i_1 b + \cdots, \quad i_\ell \in \{0, \dots, b-1\}. \quad (7b)$$

For $s \in \mathbb{N}_0$, the formula in (4) becomes

$$\begin{aligned} \tilde{f}_s(\mathbf{k}) &= \frac{1}{2^s} \sum_{i=0}^{2^s-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_i \rangle} f(\mathbf{x}_i) \\ &= \frac{1}{2^s} \sum_{j=0}^{b-1} \sum_{i=0}^{2^{s-1}-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_{i+j2^s} \rangle} f(\mathbf{x}_{i+j2^s}) \\ &= \frac{1}{b} \sum_{j=0}^{b-1} e^{-2\pi\sqrt{-1}j\langle \mathbf{k}, \mathbf{z}_s \rangle} \left[\frac{1}{2^{s-1}} \sum_{i=0}^{2^{s-1}-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_i \rangle} f(\mathbf{x}_{i+j2^s}) \right] \\ &= \mathbb{1}_{\mathcal{Z}_s^\perp}(\mathbf{k}) \left[\frac{1}{2^{s-1}} \sum_{i=0}^{2^{s-1}-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_i \rangle} f(\mathbf{x}_{i+j2^s}) \right] \end{aligned}$$

1.6. Tony

Proposition 1. For a prime base b , we have the following relationship between the coefficients for different values of s

$$\tilde{f}_{s,\kappa} = \sum_{j=0}^{2^r-1} \tilde{f}_{s+r,\kappa+j2^s} \quad (8)$$

Proof. We only have to proof that

$$\tilde{f}_{s,\kappa} = \sum_{j=0}^{b-1} \tilde{f}_{s+1,\kappa+j2^s} \quad (9)$$

The general sum is an iteration of $r - 1$ times this equality.

Remember that for $a \in \mathbb{Z}_p$ we have a^{-1} because p is prime. For $\kappa = 0, \dots, 2^s - 1$, consider $\mathcal{P}_{s,\kappa}^\perp = \{k \in \mathbb{K} : k^T[h]_s = \kappa + a2^s\}$

$$\begin{aligned} 0 &= \frac{1}{2^{s+1}} \sum_{a=1}^{b-1} \sum_{k=0}^{b-1} e^{-2\pi\sqrt{-1}\frac{k}{b}} \sum_{i=a2^s}^{(a+1)2^s-1} f(\mathbf{x}_i) e^{-2\pi\sqrt{-1}\kappa\phi_b(i)} \\ &= \sum_{a=1}^{b-1} \sum_{k=0}^{b-1} \frac{1}{2^{s+1}} \sum_{i=0}^{2^s-1} f(\mathbf{x}_{i+a2^s}) e^{-2\pi\sqrt{-1}[\kappa(\phi_b(i) + \frac{a}{2^{s+1}}) + \frac{k}{b}]} \\ &= \sum_{a=1}^{b-1} \sum_{k=0}^{b-1} \frac{1}{2^{s+1}} \sum_{i=0}^{2^s-1} f(\mathbf{x}_{i+a2^s}) e^{-2\pi\sqrt{-1}[(\phi_b(i) + \frac{a}{2^{s+1}})(\kappa + a^{-1}k2^s)]} \\ &= \sum_{j=0}^{b-1} \frac{1}{2^{s+1}} \sum_{i=2^s}^{2^{s+1}-1} f(\mathbf{x}_i) e^{-2\pi\sqrt{-1}[(\kappa+j2^s)\phi_b(i)]} \end{aligned} \quad (10)$$

Then, considering that $0 \leq \kappa < 2^s$,

$$\begin{aligned} \tilde{f}_{s,\kappa} &= b \frac{1}{2^{s+1}} \sum_{i=0}^{2^s-1} f(\mathbf{x}_i) e^{-2\pi\sqrt{-1}\kappa\phi_b(i)} \\ &= \sum_{j=0}^{b-1} \frac{1}{2^{s+1}} \sum_{i=0}^{2^s-1} f(\mathbf{x}_i) e^{-2\pi\sqrt{-1}(\kappa+j2^s)\phi_b(i)} \\ &\quad + \sum_{j=0}^{b-1} \frac{1}{2^{s+1}} \sum_{i=2^s}^{2^{s+1}-1} f(\mathbf{x}_i) e^{-2\pi\sqrt{-1}[(\kappa+j2^s)\phi_b(i)]} \\ &= \sum_{j=0}^{b-1} \tilde{f}_{s+1,\kappa+j2^s} \end{aligned} \quad (11)$$

□

Another useful equation:

$$k^T x_{i+l2^s} = k^T [h]_{s+1} \phi_b(i+lb) = k^T [h]_s \phi_b(i) + k^T [h]_{s+1} \phi_b(l) 2^{-s} = k^T x_i + k^T [h]_{s+1} l 2^{-(s+1)}$$

$$\begin{aligned} \tilde{f}_{s+1,\kappa} &= \frac{1}{2^{s+1}} \sum_{i=0}^{2^s-1} \sum_{l=0}^{b-1} f(x_{i+l2^s}) e^{-2\pi\sqrt{-1}[k^T x_i + k^T [h]_{s+1} l 2^{-(s+1)}]} \\ &= \frac{\tilde{f}_{s,\kappa}}{b} + \frac{1}{2^{s+1}} \sum_{i=0}^{2^s-1} \sum_{l=1}^{b-1} f(x_{i+l2^s}) e^{-2\pi\sqrt{-1}[k^T x_i + k^T [h]_{s+1} l 2^{-(s+1)}]} \end{aligned}$$

2. Error Estimation and an Automatic Algorithm

2.1. Wavenumber Map

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 according to the following constraints:

- Let $\mathbf{k}(0) = \mathbf{0}$.
- For any $s, \lambda \in \mathbb{N}$, $\kappa = 0, \dots, 2^s - 1$, assign $\mathbf{k}(\kappa)$ and $\mathbf{k}(\kappa + \lambda 2^s)$ such that $\mathcal{P}_{s,\mathbf{k}(\kappa)}^\perp = \mathcal{P}_{s,\mathbf{k}(\kappa+\lambda 2^s)}^\perp$.

This wavenumber map allows us to introduce a shorthand notation that facilitates the later analysis:

$$\begin{aligned} \hat{f}_\kappa &= \hat{f}(\mathbf{k}(\kappa)), \quad \kappa \in \mathbb{N}_0, \\ \tilde{f}_{s,\kappa} &= \tilde{f}(\mathbf{k}(\kappa)) \\ &= \frac{1}{2^s} \sum_{\mathbf{x} \in \mathcal{P}_{s,\Delta}} e^{-2\pi\sqrt{-1}\langle \mathbf{k}(\kappa), \mathbf{x} \rangle} f(\mathbf{x}), \quad \kappa = 0, \dots, 2^s - 1, \quad s \in \mathbb{N}, \end{aligned}$$

as defined in (4) based on the shifted nodeset $\mathcal{P}_{s,\Delta}$,

$$\mathcal{P}_{s,\kappa}^\perp = \mathcal{P}_{s,\mathbf{k}(\kappa)}^\perp, \quad \kappa = 0, \dots, 2^s - 1.$$

According to (6), it follows that

$$\begin{aligned} \tilde{f}_{s,\kappa} &= \sum_{\mathbf{l} \in \mathcal{P}_{s,\kappa}^\perp} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}(\kappa), \Delta \rangle} \\ &= \sum_{\lambda=0}^{\infty} \hat{f}_{\kappa+\lambda 2^s} e^{2\pi\sqrt{-1}\langle \mathbf{k}(\kappa+\lambda 2^s) \ominus \mathbf{k}(\kappa), \Delta \rangle} \\ &= \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda 2^s} e^{2\pi\sqrt{-1}\langle \mathbf{k}(\kappa+\lambda 2^s) \ominus \mathbf{k}(\kappa), \Delta \rangle}. \end{aligned} \tag{12}$$

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

2.2. Sums of Series Coefficients and Their Bounds

Consider the following sums of the series coefficients defined for $r, s \in \mathbb{N}$, $r \leq s$:

$$S(r) = \sum_{\kappa=2^{r-1}}^{2^r-1} |\hat{f}_\kappa|, \quad \hat{S}(r, s) = \sum_{\kappa=2^{r-1}}^{2^r-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda 2^s}|, \quad \tilde{S}(r, s) = \sum_{\kappa=2^{r-1}}^{2^r-1} |\tilde{f}_{s, \kappa}|. \quad (13)$$

These first two quantities, which involve the true series coefficients, cannot be observed, but the third one, which involves the discrete transform coefficients, can easily be observed.

We now make critical assumptions that $\hat{S}(r, s)$ and $S(s)$ can be bounded above in terms of $S(r)$, provided that r is large enough. Fix $r_* \in \mathbb{N}$. The assumptions are the following:

$$S(s) \leq \omega(s-r)S(r), \quad \hat{S}(r, s) \leq \hat{\omega}(s-r)S(r), \quad r, s \in \mathbb{N}, \quad r_* \leq r \leq s, \quad (14)$$

for some functions ω and $\hat{\omega}$ with $\lim_{s \rightarrow \infty} \omega(s) = \lim_{s \rightarrow \infty} \hat{\omega}(s) = 0$.

The reason for enforcing these assumptions only for $r \geq r_*$ is that for small r , one might have $S(r)$ coincidentally small, since it only involves 2^r coefficients, while $S(s)$ or $\hat{S}(r, s)$ is large. If $S(s)$ is large compared to $S(r)$ for some $s > r$, it means that the true series coefficients for the integrand are large for some large wavenumbers. If $\hat{S}(r, s)$ is large compared to $S(r)$ for some $s > r$, it means that the observed discrete series coefficients may not correspond well to the true coefficients.

Under this assumption, for $r, s \in \mathbb{N}$, $r_* \leq r \leq s$, it is possible to bound the sum of the true coefficients, $S(r)$, in terms of the observed sum of the discrete coefficients, $\tilde{S}(r, s)$, as follows:

$$\begin{aligned} S(r) &= \sum_{\kappa=2^{r-1}}^{2^r-1} |\hat{f}_\kappa| = \sum_{\kappa=2^{r-1}}^{2^r-1} \left| \tilde{f}_{s, \kappa} - \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda 2^s} e^{2\pi\sqrt{-1}\langle \mathbf{l}(\kappa+\lambda 2^s) \ominus \mathbf{k}(\kappa), \mathbf{\Delta} \rangle} \right| \\ &\leq \sum_{\kappa=2^{r-1}}^{2^r-1} |\tilde{f}_{s, \kappa}| + \sum_{\kappa=2^{r-1}}^{2^r-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda 2^s}| = \tilde{S}(r, s) + \hat{S}(r, s) \\ &\leq \tilde{S}(r, s) + \hat{\omega}(s-r)S(r) \\ S(r) &\leq \frac{\tilde{S}(r, s)}{1 - \hat{\omega}(s-r)} \quad \text{provided that } \hat{\omega}(s-r) < 1. \end{aligned}$$

Using this upper bound, one can then conservatively bound the error of integration using the shifted node set $\mathcal{P}_{s, \mathbf{\Delta}}$. For for $r, s \in \mathbb{N}$, $r_* \leq r \leq s$, it

follows that

$$\begin{aligned}
& \left| \int_{\mathcal{X}} f(\mathbf{x}) \, d\mathbf{x} - \frac{1}{2^s} \sum_{\mathbf{x} \in \mathcal{P}_{s, \Delta}} f(\mathbf{x}) \right| \\
&= \left| \hat{f}(\mathbf{0}) - \tilde{f}(\mathbf{0}) \right| = \left| \hat{f}_0 - \tilde{f}_{s,0} \right| = \left| \sum_{\lambda=1}^{\infty} \hat{f}_{\lambda 2^s} e^{2\pi\sqrt{-1}\langle \mathbf{l}(\lambda 2^s), \Delta \rangle} \right| \\
&\leq \sum_{\lambda=1}^{\infty} |\hat{f}_{\lambda 2^s}| \\
&\leq \sum_{\kappa=2^s}^{\infty} |\hat{f}_{\kappa}| = \sum_{r'=s+1}^{\infty} \sum_{\kappa=2^{r'}-1}^{2^{r'}-1} |\hat{f}_{\kappa}| = \sum_{r'=s+1}^{\infty} S(r') \\
&\leq \sum_{r'=s+1}^{\infty} \omega(r' - r) S(r) = \sum_{r'=1}^{\infty} \omega(r' + s - r) S(r) = \Omega(s - r) S(r) \\
&\leq \frac{\tilde{S}(r, s) \Omega(s - r)}{1 - \hat{\omega}(s - r)}.
\end{aligned}$$

where

$$\Omega(\delta) = \sum_{r'=1}^{\infty} \omega(r' + \delta), \quad \delta \in \mathbb{N}_0.$$

Assuming that $\Omega(0)$ is finite, $\lim_{\delta \rightarrow \infty} \Omega(\delta) = 0$.

This error bound suggests the following algorithm. Choose $\delta \in \mathbb{N}_0$ such that $\hat{\omega}(s - r) < 1$ and set

$$\mathfrak{C} = \frac{\Omega(\delta)}{1 - \hat{\omega}(\delta)}.$$

Define $r_j = r_* + j - 1$ and $s_j = r_j + \delta$. Given a tolerance ε , and an integrand f , do the following: for $j = 1, 2, \dots$ check whether

$$\mathfrak{C} \tilde{S}(r_j, s_j) \leq \varepsilon.$$

If so, we're done. If not, increment j by one and repeat.

$$\tilde{f} a^{\tilde{f}} a_{\tilde{f}}$$

3. Computing the fast transform efficiently

Given $i = 0, \dots, 2^m - 1$, the points generated in our nested rank-1 integration lattices can be written as $\mathbf{z}_i = \mathbf{t}_i + \Delta$, $\Delta \in [0, 1)^d$. For $i = 2^0 i_1 + 2i_2 + \dots + 2^{m-1} i_m$, we can decompose $\mathbf{t}_i = i_1 \mathbf{t}_{2^0} + i_2 \mathbf{t}_{2^1} + i_3 \mathbf{t}_{2^2} \dots + i_m \mathbf{t}_{2^{m-1}}$. This will be useful in our Fast Fourier Transform since,

$$\tilde{f}_{m, \Delta}(\mathbf{k}) = \left[\frac{1}{2^m} \sum_{i=0}^{2^m-1} f(\mathbf{z}_i) e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \rangle} \right] e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \Delta \rangle}$$

where without loosing generality we shall work with $\Delta = 0$.

Then, a mapping $\tilde{\nu}_m : \mathbb{Z}^d \rightarrow \mathbb{Z}_{2^m}$ arises naturally: for $\tilde{\nu}_m(\mathbf{k}) = \nu \in \{0, \dots, 2^m - 1\}$, we define ν such that $\langle \mathbf{k}, \mathbf{t}_{2^m-1} \rangle = \nu 2^{-m}$. Using this definition it follow that $\tilde{\nu}_m(\mathbf{k}) = \tilde{\nu}_{m-1}(\mathbf{k}) + a$, $a \in \{0, 2^{m-1}\}$, since $\langle \mathbf{k}, \mathbf{t}_{2^j-1} \rangle = (\nu \bmod 2^j) 2^{-j}$. Thus,

$$\tilde{f}_{m, \mathbf{0}}(\mathbf{k}) = \frac{1}{2^m} \sum_{i_1=0}^1 \cdots \sum_{i_m=0}^1 f(\mathbf{z}_i) e^{-2\pi\sqrt{-1}[i_1(\nu \bmod 2^1)2^{-1} + \cdots + i_m(\nu \bmod 2^m)2^{-m}]}$$

If $\nu = 2^0\nu_1 + 2\nu_2 + \cdots + 2^{m-1}\nu_m$, the mapping chosen lets us to work with $\tilde{f}_{m, \mathbf{0}}$ as a function of ν ,

$$\begin{aligned} \tilde{f}_{m, \mathbf{0}}(\nu_1, \dots, \nu_m) &= \frac{1}{2^m} \sum_{i_j=0}^1 \cdots \sum_{i_1=0}^1 f(\mathbf{z}_i) e^{-2\pi\sqrt{-1}[\sum_{l=1}^m \nu_l \sum_{j=l}^m i_j 2^{-j}]} \\ &= \frac{1}{2^m} \sum_{i_j=0}^1 \cdots \sum_{i_1=0}^1 f(\mathbf{z}_i) e^{-2\pi\sqrt{-1}[\sum_{j=1}^m i_j 2^{-j} \sum_{l=1}^j \nu_l]} \\ &= \frac{1}{2^m} \sum_{i_j=0}^1 \cdots e^{-2\pi\sqrt{-1}[\sum_{j=2}^m i_j 2^{-j} \sum_{l=1}^j \nu_l]} \sum_{i_1=0}^1 f(\mathbf{z}_i) e^{-2\pi\sqrt{-1}[i_1 2^{-1} \nu_1]} \end{aligned}$$