

Error Estimation for Cubature Based on rank-1 lattices

Fred J. Hickernell

*Room E1-208, Department of Applied Mathematics, Illinois Institute of Technology,
10 W. 32nd St., Chicago, IL 60616*

Lluís Antoni Jiménez Rugama

*Room E1-120, Department of Applied Mathematics, Illinois Institute of Technology,
10 W. 32nd St., Chicago, IL 60616*

Abstract

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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. Define \mathcal{X} to be a field with the additive operation $\oplus : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{X}$, $\mathbf{x} \oplus \mathbf{y} = \mathbf{x} + \mathbf{y} \pmod{1}$. Indeed, (\mathcal{X}, \oplus) is an Abelian group. Here $\mathbf{0}$ is the additive identity. The unique additive inverse of \mathbf{x} is $\ominus \mathbf{x} := \mathbf{1} - \mathbf{x}$, and $\mathbf{x} \ominus \mathbf{t}$ means $\mathbf{x} \oplus (\ominus \mathbf{t})$. Moreover, such a set \mathcal{X} is also a vector space under the field \mathbb{Z} and the multiplicative operation is seen by means of \oplus :

$$a\mathbf{x} := \underbrace{\mathbf{x} \oplus \cdots \oplus \mathbf{x}}_{a \text{ times}} \quad \forall a \in \mathbb{N}, \quad a\mathbf{x} := \underbrace{\ominus \mathbf{x} \ominus \cdots \ominus \mathbf{x}}_{-a \text{ times}} \quad \forall a \in \mathbb{Z} \setminus \mathbb{N}_0.$$

The set $\mathbb{K} := \mathbb{Z}^d$ is used to index series expressions for the integrands. This is a field with the natural sum and similarly to \mathcal{X} , a vector space under \mathbb{Z} .

Now, define the bilinear operation $\langle \cdot, \cdot \rangle : \mathbb{K} \times \mathcal{X} \rightarrow \mathcal{X}$,

$$\langle \mathbf{k}, \mathbf{x} \rangle = \mathbf{k}^T \mathbf{x} \pmod{1}. \quad (1a)$$

For all $\mathbf{t}, \mathbf{x} \in \mathcal{X}$, $\mathbf{k}, \mathbf{l} \in \mathbb{K}$, and $a \in \mathbb{Z}$, it follows that

$$\langle \mathbf{k}, \mathbf{0} \rangle = \langle \mathbf{0}, \mathbf{x} \rangle = 0, \quad (1b)$$

$$\langle \mathbf{k}, a\mathbf{x} \oplus \mathbf{t} \rangle = a \langle \mathbf{k}, \mathbf{x} \rangle + \langle \mathbf{k}, \mathbf{t} \rangle \pmod{1} \quad (1c)$$

$$\langle a\mathbf{k} + \mathbf{l}, \mathbf{x} \rangle = a \langle \mathbf{k}, \mathbf{x} \rangle + \langle \mathbf{l}, \mathbf{x} \rangle \pmod{1}, \quad (1d)$$

$$\langle \mathbf{k}, \mathbf{x} \rangle = 0 \quad \forall \mathbf{k} \in \mathbb{K} \implies \mathbf{x} = \mathbf{0}. \quad (1e)$$

1.2. Sequences, Nets, and Dual Nets

Suppose that there exists a sequence of points in \mathcal{X} , denoted $\mathcal{P}_\infty = \{\mathbf{t}_i\}_{i=0}^\infty$. Any $\mathcal{P}_m := \{\mathbf{t}_i\}_{i=0}^{b^m-1}$ doted with \oplus is an Abelian subgroup of \mathcal{P}_∞ . They are called *nets* and all are nested, i.e. $\{0\} = \mathcal{P}_0 \subseteq \cdots \subseteq \mathcal{P}_m \subseteq \cdots \subseteq \mathcal{P}_\infty$. Furthermore, \mathcal{P}_∞ is assumed to satisfy the following properties:

$$\{\mathbf{t}_1, \mathbf{t}_b, \mathbf{t}_{b^2}, \dots\} \text{ are linearly independent,} \quad (2a)$$

$$b\mathbf{t}_{b^m} = \mathbf{t}_{b^{m+1}}, \quad (2b)$$

$$\mathbf{t}_i = \sum_{\ell=0}^{\infty} i_\ell \mathbf{t}_{b^\ell}, \quad \text{where } \vec{i} = (i_0, i_1, i_2, \dots) \in \mathbb{F}_b^\infty, \quad (2c)$$

$$\langle \mathbf{k}, \mathbf{t}_i \rangle = 0 \ \forall i \in \mathbb{N}_0 \implies \mathbf{k} = \mathbf{0}. \quad (2d)$$

Note that from (1) together with (2b) it follows,

$$\langle \mathbf{k}, \mathbf{t}_{b^{m-1}} \rangle = \langle b\mathbf{k}, \mathbf{t}_{b^m} \rangle \quad (3)$$

One example is the extensible *rank*-1 lattices [1]. For $\mathcal{P}_m := \{\mathbf{z}_{\frac{n}{b^m}}, n \in \mathbb{F}_{b^m}\}$ the nested structure detailed above is well defined and the vector \mathbf{z} can be seen in each coordinate as an infinite digit integer. In addition, for every \mathcal{P}_m we can find a generator. If we want $\mathbf{t}_{b^{m-1}} = \mathbf{z}_{\frac{j_m}{b^m}}$ to be the generator of \mathcal{P}_m , it only suffices to verify that $\gcd(j_m, b^m) = 1$ with $j_m \in \mathbb{F}_{b^m}$. This vector $\mathbf{j} = (j_0, j_1, \dots)$ will define the choice of generators for all subgroups of the sequence \mathcal{P}_∞ . In order to satisfy (2c), note that the order of the sequence \mathcal{P}_∞ given the generators must be the Sobol order. Equation (2b) also gives us another condition on j_m 's: $b^{m-1} \mid j_m - j_{m-1} \rightarrow j_m = j_{m-1} + b^{m-1}, \forall m \in \mathbb{N}$.

For $m \in \mathbb{N}_0$ define the *dual net* corresponding to \mathcal{P}_m as

$$\begin{aligned} \mathcal{P}_m^\perp &= \{\mathbf{k} \in \mathbb{K} : \langle \mathbf{k}, \mathbf{t}_i \rangle = 0, \ i = 0, \dots, b^m - 1\} \\ &= \{\mathbf{k} \in \mathbb{K} : \langle \mathbf{k}, \mathbf{t}_{b^\ell} \rangle = 0, \ \ell = 0, \dots, m - 1\}. \end{aligned}$$

By this definition $\mathcal{P}_0^\perp = \mathbb{K}$. The properties of the bilinear transform, (1), imply that the dual net \mathcal{P}_m^\perp is a subgroup, and even a subspace, of the dual net \mathcal{P}_ℓ^\perp for all $\ell = 0, \dots, m - 1$.

The next goal is to define the map $\hat{\nu} : \mathbb{K} \rightarrow \mathbb{F}_b^\infty$, and $\tilde{\nu}_m : \mathbb{K} \rightarrow \mathbb{F}_{b^m}$ that facilitates the calculation of the discrete Fourier transform introduced below.

Definition 1. For every $\mathbf{k} \in \mathbb{K}$, let

$$\hat{\nu}(\mathbf{k}) = (\hat{\nu}_0(\mathbf{k}), \hat{\nu}_1(\mathbf{k}), \hat{\nu}_2(\mathbf{k}), \dots), \quad (4a)$$

$$\hat{\nu}_0(\mathbf{k}) = b \langle \mathbf{k}, \mathbf{t}_1 \rangle, \quad \hat{\nu}_m(\mathbf{k}) = b \langle \mathbf{k}, \mathbf{t}_{b^m} \rangle - \langle \mathbf{k}, \mathbf{t}_{b^{m-1}} \rangle, \quad m \in \mathbb{N}, \quad (4b)$$

$$\tilde{\nu}_m(\mathbf{k}) = \sum_{\ell=0}^{m-1} \hat{\nu}_\ell(\mathbf{k}) b^\ell, \quad m \in \mathbb{N}. \quad (4c)$$

These maps have certain desirable properties.

Lemma 1. *The following is true for the maps defined in Definition 1:*

- a) $\widehat{\nu}(\mathbf{0}) = \mathbf{0}$ and $\tilde{\nu}_m(\mathbf{0}) = 0$ for all $m \in \mathbb{N}$.
- b) $\hat{\nu}_m(\mathbf{k}) \in \{0, \dots, b-1\}$ and $\tilde{\nu}_m(\mathbf{k}) \in \{0, \dots, b^m - 1\}$ for all $m \in \mathbb{N}_0$.
- c) for all $m \in \mathbb{N}_0$ and all $\boldsymbol{\nu} \in \mathbb{F}_b^m$ there exist a unique $\mathbf{k} \in \mathbb{K}$ with $\widehat{\nu}(\mathbf{k}) = (\nu_0, \dots, \nu_{m-1}, \dots)$.
- d) for any $m \in \mathbb{N}_0$, $i \in \{0, \dots, b^m - 1\}$, $\tilde{\nu}_m(\mathbf{k}) = \nu = (\nu_0, \nu_1, \dots)$, and $\vec{i} = (i_0, i_1, \dots)$, it follows that

$$\langle \mathbf{k}, \mathbf{t}_i \rangle = \sum_{\ell=0}^{m-1} i_\ell \sum_{j=0}^{\ell} \nu_j b^{j-(\ell+1)} \pmod{1} \quad (5)$$

Proof. a) Directly from definition.

- b) Using (2c) and by construction, $\hat{\nu}_0(\mathbf{k}) \in \{0, \dots, b-1\}$ and $\hat{\nu}_m(\mathbf{k}) \in (-1, b)$. Using the assumption (2b), $\hat{\nu}_m(\mathbf{k}) \pmod{1} = \mathbf{k}^T b \mathbf{t}_{b^m} \pmod{1} - \mathbf{k}^T \mathbf{t}_{b^{m-1}} \pmod{1} = 0$. Then, $\hat{\nu}_m(\mathbf{k}) \in (-1, b) \cap \mathbb{Z} = \{0, \dots, b-1\}, \forall m \in \mathbb{N}_0$.
- c) For injectivity, we prove that $\widehat{\nu}(\mathbf{k}) = \widehat{\nu}(\mathbf{l}) \Rightarrow \mathbf{k} = \mathbf{l}$. If $\widehat{\nu}(\mathbf{k}) = \widehat{\nu}(\mathbf{l})$, $\hat{\nu}_m(\mathbf{k}) = \hat{\nu}_m(\mathbf{l}), \forall m \in \mathbb{N}_0$. In particular for $m = 0$, this implies $\langle \mathbf{k}, \mathbf{t}_1 \rangle - \langle \mathbf{l}, \mathbf{t}_1 \rangle = 0$. Assume now that $\langle \mathbf{k}, \mathbf{t}_{b^m} \rangle - \langle \mathbf{l}, \mathbf{t}_{b^m} \rangle = 0$. Since $\hat{\nu}_{m+1}(\mathbf{k}) - \hat{\nu}_{m+1}(\mathbf{l}) = 0$, then $\langle \mathbf{k}, \mathbf{t}_{b^{m+1}} \rangle - \langle \mathbf{l}, \mathbf{t}_{b^{m+1}} \rangle = 0$. By induction $\langle \mathbf{k}, \mathbf{t}_{b^m} \rangle - \langle \mathbf{l}, \mathbf{t}_{b^m} \rangle = \langle \mathbf{k} - \mathbf{l}, \mathbf{t}_{b^m} \rangle = 0$ for all $m \in \mathbb{N}_0$. Thus, by (2d), $\mathbf{k} = \mathbf{l}$.

For the surjection, by (1e) there exists \mathbf{k} such that $\hat{\nu}_0(\mathbf{k}) = \nu \neq 0$. Furthermore due to the property (1d), $\hat{\nu}_0(a\mathbf{k}) = a\nu \pmod{b}$ and recalling the Lagrange's Theorem, any element ν different of the identity generates the group \mathbb{F}_b . Therefore, $a = 1, \dots, b-1$ gives us any element of \mathbb{F}_b .

Now, for any $l \leq m \in \mathbb{N}$ and using (3),

$$\begin{aligned} \hat{\nu}_l(\mathbf{k} + b^m \mathbf{a}) &= \begin{cases} b \langle \mathbf{k}, \mathbf{t}_{b^l} \rangle - \langle \mathbf{k}, \mathbf{t}_{b^{l-1}} \rangle + b \langle \mathbf{a}, \mathbf{t}_1 \rangle & \pmod{b} \quad \text{if } l = m, \\ b \langle \mathbf{k}, \mathbf{t}_{b^l} \rangle - \langle \mathbf{k}, \mathbf{t}_{b^{l-1}} \rangle & \text{if } l < m \end{cases} \\ &= \begin{cases} \hat{\nu}_l(\mathbf{k}) + \hat{\nu}_0(\mathbf{a}) & \pmod{b} \quad \text{if } l = m, \\ \hat{\nu}_l(\mathbf{k}) & \text{if } l < m \end{cases} \end{aligned}$$

Therefore, for all $m \in \mathbb{N}_0$ and all $(\nu_0, \dots, \nu_m) \in \mathbb{F}_b^{m+1}$ there exist a $\mathbf{k} \in \mathbb{K}$ with $\hat{\nu}_l(\mathbf{k}) = \nu_l, l = 0, \dots, m$. This means $\widehat{\nu}(\mathbf{k})$ is bijective.

- d) Follows by applying (1c) and Definition 1:

$$\begin{aligned} \langle \mathbf{k}, \mathbf{t}_i \rangle &= \left\langle \mathbf{k}, \sum_{\ell=0}^{m-1} i_\ell \mathbf{t}_{b^\ell} \right\rangle = \sum_{\ell=0}^{m-1} i_\ell \langle \mathbf{k}, \mathbf{t}_{b^\ell} \rangle \pmod{1} \\ &= \sum_{\ell=0}^{m-1} i_\ell \sum_{j=0}^{\ell} \nu_j b^{j-(\ell+1)} \pmod{1}. \end{aligned}$$

□

1.3. Fourier Walsh Series and Discrete Transforms

The integrands are assumed to belong to some subset of $\mathcal{L}_2([0, 1]^d)$, the space of square integrable functions. The \mathcal{L}_2 inner product is defined as

$$\langle f, g \rangle_2 = \int_{[0, 1]^d} f(\mathbf{x}) \overline{g(\mathbf{x})} d\mathbf{x}.$$

Let $\{\varphi(\cdot, \mathbf{k}) \in \mathcal{L}_2([0, 1]^d) : \mathbf{k} \in \mathbb{K}\}$ be the complete orthonormal Walsh function *basis* for $\mathcal{L}_2([0, 1]^d)$, i.e.,

$$\varphi(\mathbf{x}, \mathbf{k}) = e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle / b}, \quad \mathbf{k} \in \mathbb{K}, \quad \mathbf{x} \in [0, 1]^d.$$

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

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{K}} \hat{f}(\mathbf{k}) \varphi(\mathbf{x}, \mathbf{k}), \quad \text{where } \hat{f}(\mathbf{k}) = \langle f, \varphi(\cdot, \mathbf{k}) \rangle_2, \quad (6)$$

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

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

For all $\mathbf{k} \in \mathbb{K}$ and $\mathbf{x} \in \mathcal{P}$, it follows that

$$\begin{aligned} 0 &= \frac{1}{b^m} \sum_{i=0}^{b^m-1} [\varphi(\mathbf{t}_i, \mathbf{k}) - \varphi(\mathbf{t}_i \oplus \mathbf{x}, \mathbf{k})] = \frac{1}{b^m} \sum_{i=0}^{b^m-1} [e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \rangle} - e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \oplus \mathbf{x} \rangle}] \\ &= \frac{1}{b^m} \sum_{i=0}^{b^m-1} [e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \rangle} - e^{2\pi\sqrt{-1}\{\langle \mathbf{k}, \mathbf{t}_i \rangle + \langle \mathbf{k}, \mathbf{x} \rangle\}}] \quad \text{by (1c)} \\ &= [1 - e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle}] \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \rangle}. \end{aligned}$$

By this equality 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.

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

Given the digital sequence $\{\mathbf{t}_i\}_{i=0}^\infty$, one may also define a digitally shifted sequence $\{\mathbf{x}_i = \mathbf{t}_i \oplus \mathbf{\Delta}\}_{i=0}^\infty$, where $\mathbf{\Delta} \in [0, 1]^d$. Suppose that $\text{trail}(\mathbf{t}_i, \mathbf{\Delta}) = \infty$ for all $i \in \mathbb{N}_0$. Define the discrete transform of a function, f , over the shifted

net as

$$\begin{aligned}
\tilde{f}_m(\mathbf{k}) &:= \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_i \rangle / b} f(\mathbf{x}_i) \\
&= \frac{1}{b^m} \sum_{i=0}^{b^m-1} \left[e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_i \rangle / b} \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l}, \mathbf{x}_i \rangle / b} \right] \\
&= \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \mathbf{x}_i \rangle / b} \\
&= \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \Delta \rangle / b} \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \mathbf{t}_i \rangle / b} \\
&= \sum_{\mathbf{l} \in \mathbb{K}} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \Delta \rangle / b} \mathbb{1}_{\mathcal{P}_m^\perp}(\mathbf{l} \ominus \mathbf{k}) \\
&= \sum_{\mathbf{l} \in \mathcal{P}_m^\perp} \hat{f}(\mathbf{k} \oplus \mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l}, \Delta \rangle / b} \\
&= \hat{f}(\mathbf{k}) + \sum_{\mathbf{l} \in \mathcal{P}_m^\perp \setminus \mathbf{0}} \hat{f}(\mathbf{k} \oplus \mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l}, \Delta \rangle / b}, \quad \forall \mathbf{k} \in \mathbb{K}.
\end{aligned} \tag{7}$$

It is seen here that the discrete transform $\tilde{f}_m(\mathbf{k})$ is equal to the integral transform $\hat{f}(\mathbf{k})$, defined in (6), plus the *aliasing* terms corresponding to $\hat{f}(\mathbf{l})$ where $\mathbf{l} \ominus \mathbf{k} \in \mathcal{P}_m^\perp \setminus \mathbf{0}$.

1.4. Computation of the Discrete Transform

The discrete transform defined in (7) may also be expressed as

$$\begin{aligned}
\tilde{f}_m(\mathbf{k}) &= \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \oplus \Delta \rangle / b} f(\mathbf{t}_i \oplus \Delta) \\
&= \frac{e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \Delta \rangle / b}}{b^m} \sum_{i=0}^{b^m-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \rangle / b} f(\mathbf{t}_i \oplus \Delta).
\end{aligned}$$

Letting $y_i = f(\mathbf{t}_i \oplus \Delta)$,

$$Y_{m,0}(i_0, \dots, i_{m-1}) = y_i, \quad i = i_0 + i_1 b + \dots + i_{m-1} b^{m-1},$$

and invoking Lemma 1, for any $\mathbf{k} \in \mathbb{K}$ with $\tilde{\nu}_m(\mathbf{k}) = \nu = \nu_0 + \nu_1 b + \dots + \nu_{m-1} b^{m-1}$ one may write

$$\begin{aligned}
\tilde{f}_m(\mathbf{k}) &= e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \Delta \rangle / b} Y_{m,m}(\nu_0, \dots, \nu_{m-1}), \\
Y_{m,m}(\nu_0, \dots, \nu_{m-1}) &:= \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \rangle / b} y_i \\
&= \frac{1}{b^m} \sum_{i_{m-1}=0}^{b-1} \dots \sum_{i_0=0}^{b-1} e^{-2\pi\sqrt{-1} \sum_{\ell=0}^{m-1} \nu_\ell i_\ell / b} Y_{m,0}(i_1, \dots, i_m) \\
&= \frac{1}{b} \sum_{i_{m-1}=0}^{b-1} e^{-2\pi\sqrt{-1} \nu_{m-1} i_{m-1} / b} \dots \\
&\quad \frac{1}{b} \sum_{i_0=0}^{b-1} e^{-2\pi\sqrt{-1} \nu_0 i_0 / b} Y_{m,0}(i_1, \dots, i_m)
\end{aligned}$$

This sum can be computed recursively:

$$\begin{aligned}
Y_{m,\ell+1}(\nu_0, \dots, \nu_\ell, i_{\ell+1}, \dots, i_m) \\
= \frac{1}{b} \sum_{i_\ell=0}^{b-1} e^{-2\pi\sqrt{-1} \nu_\ell i_\ell / b} Y_{m,\ell}(\nu_1, \dots, \nu_{\ell-1}, i_\ell, \dots, i_m)
\end{aligned}$$

In light of this development we define $\mathring{f}_m(\nu) = Y_{m,m}(\nu_0, \dots, \nu_{m-1})$ for $\nu = 0, \dots, b^m - 1$. Then

$$\tilde{f}(\mathbf{k}) = e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \Delta \rangle / b} \mathring{f}_m(\tilde{\nu}(\mathbf{k})).$$

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 $\tilde{\mathbf{k}}(\kappa) \in \mathbb{K}$ iteratively according to the following constraints:

- i) $\tilde{\mathbf{k}}(0) = \mathbf{0}$;
- ii) For any $\lambda, m \in \mathbb{N}_0$ and $\kappa = 0, \dots, b^m - 1$, it follows that $\tilde{\nu}_m(\tilde{\mathbf{k}}(\kappa)) = \tilde{\nu}_m(\tilde{\mathbf{k}}(\kappa + \lambda b^m))$.

This last condition implies that $\tilde{\mathbf{k}}(\kappa) \ominus \tilde{\mathbf{k}}(\kappa + \lambda b^m) \in \mathcal{P}_m^\perp$.

This wavenumber map allows us to introduce a shorthand notation that facilitates the later analysis for $\kappa \in \mathbb{N}_0$ and $m \in \mathbb{N}$:

$$\begin{aligned}
\hat{f}_\kappa &= \hat{f}(\tilde{\mathbf{k}}(\kappa)), \\
\tilde{f}_{m,\kappa} &= \tilde{f}_m(\tilde{\mathbf{k}}(\kappa)) = e^{-2\pi\sqrt{-1}\langle \tilde{\mathbf{k}}(\kappa), \Delta \rangle / b} \mathring{f}_m(\tilde{\nu}_m(\tilde{\mathbf{k}}(\kappa))) \\
&= e^{-2\pi\sqrt{-1}\langle \tilde{\mathbf{k}}(\kappa), \Delta \rangle / b} \mathring{f}_m(\tilde{\nu}_m(\kappa)),
\end{aligned}$$

where $\hat{\nu}_m(\kappa) := \tilde{\nu}_m(\tilde{\mathbf{k}}(\kappa))$. According to (8), it follows that

$$\tilde{f}_{m,\kappa} = \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda b^m} e^{2\pi\sqrt{-1}\langle \tilde{\mathbf{k}}(\kappa+\lambda b^m) \ominus \tilde{\mathbf{k}}(\kappa), \Delta \rangle / b}. \quad (9)$$

We want to use $\tilde{f}_{m,\kappa}$ to estimate \hat{f}_κ if m 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 $\ell, m \in \mathbb{N}$, $\ell \leq m$:

$$\begin{aligned} S(m) &= \sum_{\kappa=b^{m-1}}^{b^m-1} |\hat{f}_\kappa|, & \hat{S}(\ell, m) &= \sum_{\kappa=b^{\ell-1}}^{b^\ell-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda b^m}|, \\ \tilde{S}(\ell, m) &= \sum_{\kappa=b^{\ell-1}}^{b^\ell-1} |\tilde{f}_{m,\kappa}| = \sum_{\kappa=b^{\ell-1}}^{b^\ell-1} |\hat{f}_m(\hat{\nu}(\kappa))|. \end{aligned}$$

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 $\hat{S}(\ell, m)$ and $S(m)$ can be bounded above in terms of $S(\ell)$, provided that ℓ is large enough. Fix $\ell_* \in \mathbb{N}$. The assumptions are the following:

$$S(m) \leq \omega(m - \ell) S(\ell), \quad \hat{S}(\ell, m) \leq \hat{\omega}(m - \ell) S(\ell), \quad \ell, m \in \mathbb{N}, \ell_* \leq \ell \leq m, \quad (10)$$

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

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

Under this assumption, for $\ell, s \in \mathbb{N}$, $\ell_* \leq \ell \leq s$, it is possible to bound the sum of the true coefficients, $S(\ell)$, in terms of the observed sum of the discrete

coefficients, $\tilde{S}(\ell, s)$, as follows:

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

Using this upper bound, one can then conservatively bound the error of integration using the shifted node set. For $\ell, m \in \mathbb{N}$, $\ell_* \leq \ell \leq m$, it follows that

$$\begin{aligned}
&\left| \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} - \frac{1}{b^m} \sum_{i=0}^{b^m-1} f(\mathbf{x}) \right| \\
&= \left| \hat{f}(\mathbf{0}) - \tilde{f}_m(\mathbf{0}) \right| = \left| \hat{f}_0 - \tilde{f}_{m,0} \right| = \left| \sum_{\lambda=1}^{\infty} \hat{f}_{\lambda b^s} e^{2\pi\sqrt{-1}\mathbf{l}(\lambda b^s) \otimes \mathbf{\Delta}} \right| \\
&\leq \sum_{\lambda=1}^{\infty} |\hat{f}_{\lambda b^m}| \\
&\leq \sum_{\kappa=b^m}^{\infty} |\hat{f}_\kappa| = \sum_{r=m+1}^{\infty} \sum_{\kappa=b^{r-1}}^{b^r-1} |\hat{f}_\kappa| = \sum_{r=m+1}^{\infty} S(r) \\
&\leq \sum_{r=s+1}^{\infty} \omega(r - \ell) S(\ell) = \sum_{r=1}^{\infty} \omega(r + m - \ell) S(\ell) = \Omega(m - \ell) S(\ell) \\
&\leq \frac{\tilde{S}(\ell, m) \Omega(m - \ell)}{1 - \hat{\omega}(m - \ell)}.
\end{aligned}$$

where

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

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

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

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

Define $\ell_j = \ell_* + j - 1$ and $m_j = \ell_j + r$. Given a tolerance ε , and an integrand f , do the following: for $j = 1, 2, \dots$ check whether

$$\mathfrak{C} \tilde{S}(\ell_j, m_j) \leq \varepsilon.$$

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

- [1] F. J. Hickernell and H. Niederreiter, “The existence of good extensible rank-1 lattices,” *J. Complexity*, vol. 19, pp. 286–300, 2003.