Error Estimation for Cubature Based on rank-1 lattices

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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 $\oplus : \mathcal{X} \times \mathcal{X} \to \mathcal{X}$, $\boldsymbol{x} \oplus \boldsymbol{y} = \boldsymbol{x} + \boldsymbol{y} \pmod 1$. Indeed, $(\mathcal{X}, \oplus)$ is an Abelian group. Here $\mathbf{0}$ is the additive identity. The unique additive inverse of $\boldsymbol{x}$ is $\ominus \boldsymbol{x} := \mathbf{1} - \boldsymbol{x}$, and $\boldsymbol{x} \ominus \boldsymbol{t}$ means $\boldsymbol{x} \oplus (\ominus \boldsymbol{t})$. 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 $\oplus$:

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

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 multiplication. Similarly to $\mathcal{X}$, it is also a vector space under $\mathbb{Z}$.

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

$$\langle \boldsymbol{k}, \boldsymbol{x} \rangle = \boldsymbol{k}^T \boldsymbol{y} \pmod 1. \tag{1a}$$

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

$$\langle \boldsymbol{k}, \mathbf{0} \rangle = \langle \mathbf{0}, \boldsymbol{x} \rangle = 0, \tag{1b}$$

$$\langle \boldsymbol{k}, a\boldsymbol{x} \oplus \boldsymbol{t} \rangle = a \langle \boldsymbol{k}, \boldsymbol{x} \rangle + \langle \boldsymbol{k}, \boldsymbol{t} \rangle \pmod 1 \tag{1c}$$

$$\langle a\boldsymbol{k} + \boldsymbol{l}, \boldsymbol{x} \rangle = a \langle \boldsymbol{k}, \boldsymbol{x} \rangle + \langle \boldsymbol{l}, \boldsymbol{x} \rangle \pmod 1, \tag{1d}$$

$$\langle \boldsymbol{k}, \boldsymbol{x} \rangle = 0 \ \forall \boldsymbol{k} \in \mathbb{K} \Longrightarrow \boldsymbol{x} = \mathbf{0}. \tag{1e}$$

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1.2. Sequences, Nets, and Dual Nets

Suppose that there exists a sequence of points in $\mathcal{X}$, denoted $\mathcal{P}_\infty = \{\boldsymbol{t}_i\}_{i=0}^{\infty}$. Any $\mathcal{P}_m := \{\boldsymbol{t}_i\}_{i=0}^{b^m-1}$ doted with $\oplus$ is an Abelian subgroup of $\mathcal{P}_\infty$. 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, $\mathcal{P}_\infty$ is assumed to satisfy the following properties:

$$\{\boldsymbol{t}_1, \boldsymbol{t}_b, \boldsymbol{t}_{b^2}, \ldots\} \text{ are linearly independent,} \tag{2a}$$

$$b\boldsymbol{t}_{b^m} = \boldsymbol{t}_{b^{m-1}}, \tag{2b}$$

$$\boldsymbol{t}_i = \sum_{\ell=0}^{\infty} i_\ell \boldsymbol{t}_{b^\ell}, \qquad \text{where } \vec{\imath} = (i_0, i_1, i_2, \ldots) \in \mathbb{F}_b^\infty, \tag{2c}$$

$$\langle \boldsymbol{k}, \boldsymbol{t}_i \rangle = 0 \ \forall i \in \mathbb{N}_0 \Longrightarrow \boldsymbol{k} = \boldsymbol{0}. \tag{2d}$$

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

$$\langle \boldsymbol{k}, \boldsymbol{t}_{b^{m-1}} \rangle = \langle b\boldsymbol{k}, \boldsymbol{t}_{b^m} \rangle \tag{3}$$

One example is the extensible $rank{-}1$ lattices [1]. For $\mathcal{P}_m := \left\{\boldsymbol{z}\frac{n}{b^m},\ n \in \mathbb{F}_{b^m}\right\}$ the nested structure detailed above is well defined and the vector $\boldsymbol{z}$ 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 $\boldsymbol{t}_{b^{m-1}} = \boldsymbol{z}\frac{j_m}{b^m}$ to the 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 $\boldsymbol{j} = (j_0, j_1, \ldots)$ will define the choice of generators for all subgroups of the sequence $\mathcal{P}_\infty$. In order to satisfy (2c), note that the order of the sequence $\mathcal{P}_\infty$ given the generators must be the Sobol order. Equation (2b) also gives us another condition on j_m's: $b^{m-1} \mid j_m - j_{m-1} \to j_m = j_{m-1} + b^{m-1}, \forall m \in \mathbb{N}$.

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

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

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 $\mathcal{P}_\ell^\perp$ for all $\ell = 0, \ldots, m-1$.

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

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

$$\hat{\boldsymbol{\nu}}(\boldsymbol{k}) = (\hat{\nu}_0(\boldsymbol{k}), \hat{\nu}_1(\boldsymbol{k}), \hat{\nu}_2(\boldsymbol{k}), \ldots), \tag{4a}$$

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

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

These maps have certain desirable properties.

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

a) $\hat{\boldsymbol{\nu}}(\mathbf{0}) = \mathbf{0}$ *and* $\tilde{\nu}_m(\mathbf{0}) = 0$ *for all* $m \in \mathbb{N}$.

b) $\hat{\nu}_m(\boldsymbol{k}) \in \{0, \ldots, b-1\}$ *and* $\tilde{\nu}_m(\boldsymbol{k}) \in \{0, \ldots, b^m - 1\}$ *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* $\boldsymbol{k} \in \mathbb{K}$ *with* $\hat{\boldsymbol{\nu}}(\boldsymbol{k}) = (\nu_0, \ldots, \nu_{m-1}, \ldots)$.

d) *for any* $m \in \mathbb{N}_0$, $i \in \{0, \ldots, b^m - 1\}$, $\tilde{\nu}_m(\boldsymbol{k}) = \nu = (\nu_0, \nu_1, \ldots)$, *and* $\vec{\imath} = (i_0, i_1, \ldots)$, *it follows that*

$$\langle \boldsymbol{k}, \boldsymbol{t}_i \rangle = \sum_{\ell=0}^{m-1} i_\ell [\nu \pmod{b^{(\ell+1)}}] b^{-(\ell+1)} \pmod 1 \tag{5}$$

Proof. a) Directly from definition.

b) Using (2c) and by construction, $\hat{\nu}_0(\boldsymbol{k}) \in \{0, \ldots, b-1\}$ and $\hat{\nu}_m(\boldsymbol{k}) \in (-1, b)$. Using the assumption (2b), $\hat{\nu}_m(\boldsymbol{k}) \pmod 1 = \boldsymbol{k}^T b \boldsymbol{t}_{b^m} \pmod 1 - \boldsymbol{k}^T \boldsymbol{t}_{b^{m-1}} \pmod 1 = 0$. Then, $\hat{\nu}_m(\boldsymbol{k}) \in (-1, b) \cap \mathbb{Z} = \{0, \ldots, b-1\}, \forall m \in \mathbb{N}_0$.

c) For injectivity, we prove that $\hat{\boldsymbol{\nu}}(\boldsymbol{k}) = \hat{\boldsymbol{\nu}}(\boldsymbol{l}) \Rightarrow \boldsymbol{k} = \boldsymbol{l}$. If $\hat{\boldsymbol{\nu}}(\boldsymbol{k}) = \hat{\boldsymbol{\nu}}(\boldsymbol{l})$, $\hat{\nu}_m(\boldsymbol{k}) = \hat{\nu}_m(\boldsymbol{l}), \forall m \in \mathbb{N}_0$. In particular for $m = 0$, this implies $\langle \boldsymbol{k}, \boldsymbol{t}_1 \rangle - \langle \boldsymbol{l}, \boldsymbol{t}_1 \rangle = 0$. Assume now that $\langle \boldsymbol{k}, \boldsymbol{t}_{b^m} \rangle - \langle \boldsymbol{l}, \boldsymbol{t}_{b^m} \rangle = 0$. Since $\hat{\nu}_{m+1}(\boldsymbol{k}) - \hat{\nu}_{m+1}(\boldsymbol{l}) = 0$, then $\langle \boldsymbol{k}, \boldsymbol{t}_{b^{m+1}} \rangle - \langle \boldsymbol{l}, \boldsymbol{t}_{b^{m+1}} \rangle = 0$. By induction $\langle \boldsymbol{k}, \boldsymbol{t}_{b^m} \rangle - \langle \boldsymbol{l}, \boldsymbol{t}_{b^m} \rangle = \langle \boldsymbol{k} - \boldsymbol{l}, \boldsymbol{t}_{b^m} \rangle = 0$ for all $m \in \mathbb{N}_0$. Thus, by (2d), $\boldsymbol{k} = \boldsymbol{l}$.

For the surjection, by (1e) there exists $\boldsymbol{k}$ such that $\hat{\nu}_0(\boldsymbol{k}) = \nu \neq 0$. Furthermore due to the property (1d), $\hat{\nu}_0(a\boldsymbol{k}) = a\nu \pmod b$ and recalling the Lagrange's Theorem, any element ν different of the identity generates the group $\mathbb{F}_b$. Therefore, $a = 1, ..., b-1$ gives us any element of $\mathbb{F}_b$.
Now, for any $l \leqslant m \in \mathbb{N}$ and using (3),

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

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

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

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

$\square$

1.3. Fourier 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

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

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

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

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

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

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

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

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

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

By this equality 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.

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

Given the sequence $\{\boldsymbol{t}_i\}_{i=0}^\infty$, one may also define a shifted sequence $\{\boldsymbol{x}_i = \boldsymbol{t}_i \oplus \boldsymbol{\Delta}\}_{i=0}^\infty$, where $\boldsymbol{\Delta} \in [0,1)^d$. Define the discrete transform of a function, f, over the shifted net as

$$\tilde{f}_m(\boldsymbol{k}) := \frac{1}{b^m}\sum_{i=0}^{b^m-1} \mathrm{e}^{-2\pi\sqrt{-1}\langle \boldsymbol{k},\boldsymbol{x}_i\rangle} f(\boldsymbol{x}_i) \tag{7}$$

$$\begin{aligned}
&= \frac{1}{b^m}\sum_{i=0}^{b^m-1}\left[\mathrm{e}^{-2\pi\sqrt{-1}\langle \boldsymbol{k},\boldsymbol{x}_i\rangle}\sum_{\boldsymbol{l}\in\mathbb{K}}\hat{f}(\boldsymbol{l})\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l},\boldsymbol{x}_i\rangle}\right]\\
&= \sum_{\boldsymbol{l}\in\mathbb{K}}\hat{f}(\boldsymbol{l})\frac{1}{b^m}\sum_{i=0}^{b^m-1}\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}-\boldsymbol{k},\boldsymbol{x}_i\rangle}\\
&= \sum_{\boldsymbol{l}\in\mathbb{K}}\hat{f}(\boldsymbol{l})\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}-\boldsymbol{k},\boldsymbol{\Delta}\rangle}\frac{1}{b^m}\sum_{i=0}^{b^m-1}\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}-\boldsymbol{k},\boldsymbol{t}_i\rangle}\\
&= \sum_{\boldsymbol{l}\in\mathbb{K}}\hat{f}(\boldsymbol{l})\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}-\boldsymbol{k},\boldsymbol{\Delta}\rangle}\mathbb{1}_{\mathcal{P}_m^\perp}(\boldsymbol{l}-\boldsymbol{k})\\
&= \sum_{\boldsymbol{l}\in\mathcal{P}_m^\perp}\hat{f}(\boldsymbol{k}+\boldsymbol{l})\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l},\boldsymbol{\Delta}\rangle}\\
&= \hat{f}(\boldsymbol{k}) + \sum_{\boldsymbol{l}\in\mathcal{P}_m^\perp\backslash\boldsymbol{0}}\hat{f}(\boldsymbol{k}+\boldsymbol{l})\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l},\boldsymbol{\Delta}\rangle}, \qquad \forall \boldsymbol{k}\in\mathbb{K}.
\end{aligned} \tag{8}$$

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

1.4. Computation of the Discrete Transform

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

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

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

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

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

$$\begin{aligned}
\tilde{f}_m(\boldsymbol{k}) &= \mathrm{e}^{-2\pi\sqrt{-1}\langle \boldsymbol{k},\boldsymbol{\Delta}\rangle} Y_{m,m}(\nu_0,\ldots,\nu_{m-1}),\\
Y_{m,m}&(\nu_0,\ldots,\nu_{m-1})\\
&:= \frac{1}{b^m}\sum_{i=0}^{b^m-1} \mathrm{e}^{-2\pi\sqrt{-1}\langle \boldsymbol{k},\boldsymbol{t}_i\rangle} y_i\\
&= \frac{1}{b^m}\sum_{i_{m-1}=0}^{b-1}\cdots\sum_{i_0=0}^{b-1} \mathrm{e}^{-2\pi\sqrt{-1}\sum_{\ell=0}^{m-1} i_\ell [\nu \pmod{b^{(\ell+1)}}] b^{-(\ell+1)}} Y_{m,0}(i_0,\ldots,i_{m-1})\\
&= \frac{1}{b}\sum_{i_{m-1}=0}^{b-1} \mathrm{e}^{-2\pi\sqrt{-1} i_{m-1}[\nu \pmod{b^m}] b^{-m}} \cdots\\
&\qquad \frac{1}{b}\sum_{i_0=0}^{b-1} \mathrm{e}^{-2\pi\sqrt{-1} i_0[\nu \pmod{b}] b^{-1}} Y_{m,0}(i_0,\ldots,i_{m-1})
\end{aligned}$$

This sum can be computed recursively:

$$\begin{aligned}
&Y_{m,\ell+1}(\nu_0,\ldots,\nu_\ell,i_{\ell+1},\ldots,i_m)\\
&\qquad = \frac{1}{b}\sum_{i_\ell=0}^{b-1} \mathrm{e}^{-2\pi\sqrt{-1} i_\ell [\nu \pmod{b^{(\ell+1)}}] b^{-(\ell+1)}} Y_{m,\ell}(\nu_0,\ldots,\nu_{\ell-1},i_\ell,\ldots,i_m)
\end{aligned}$$

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

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

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

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

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

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

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

where $\mathring{f}_{m,\kappa} := \mathring{f}_m(\tilde{\nu}_m(\tilde{\boldsymbol{k}}(\kappa)))$. According to (8), it follows that

$$\tilde{f}_{m,\kappa} = \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda b^m} \mathrm{e}^{2\pi\sqrt{-1}\left\langle \tilde{\boldsymbol{k}}(\kappa+\lambda b^m)-\tilde{\boldsymbol{k}}(\kappa), \boldsymbol{\Delta} \right\rangle}. \tag{9}$$

We want to use $\tilde{f}_{m,\kappa}$ to estimate $\hat{f}_\kappa$ if m is signficantly 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 $\ell, m \in \mathbb{N}_0$, $\ell \leqslant m$:

$$S(m) = \sum_{\kappa=\lfloor b^{m-1} \rfloor}^{b^m-1} \left|\hat{f}_\kappa\right|, \qquad \widehat{S}(\ell, m) = \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} \sum_{\lambda=1}^{\infty} \left|\hat{f}_{\kappa+\lambda b^m}\right|,$$
$$\check{S}(m) = \widehat{S}(0, m) + \cdots + \widehat{S}(m, m) = \sum_{\kappa=b^m}^{\infty} \left|\hat{f}_\kappa\right|,$$
$$\widetilde{S}(\ell, m) = \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} \left|\tilde{f}_{m,\kappa}\right| = \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} \left|\mathring{f}_{m,\kappa}\right|.$$

The first three kinds of sums, $S(\cdot)$, $\widehat{S}(\cdot,\cdot)$, and $\check{S}(\cdot)$, which involve the true series coefficients, cannot be observed, but the last one, $\widetilde{S}(\cdot,\cdot)$, which involves the discrete transform coefficients, can easily be observed.

We now make critical assumptions that $\widehat{S}(\ell, m)$ and $\check{S}(m)$ can be bounded above in terms of $S(\ell)$, provided that ℓ is large enough. Let $\ell, m \in \mathbb{N}_0$ with $\ell \leqslant m$, and fix $\ell_* \in \mathbb{N}$. It is assumed that their exist known, non-negative valued functions $\widehat{\omega}$ and $\check{\omega}$ with $\lim_{m\to\infty} \check{\omega}(m) = 0$ such that

$$\widehat{S}(\ell, m) \leqslant \widehat{\omega}(m-\ell)\check{S}(m) \quad \forall \ell, \qquad \check{S}(m) \leqslant \check{\omega}(m-\ell)S(\ell) \quad \forall \ell_* \leqslant \ell. \tag{10}$$

By the definition of $\check{S}(m)$, the choice $\widehat{\omega}(m) := 1$ for all m is always guaranteed to work. However, one might also consider choosing $\widehat{\omega}(m) = Cb^{-m}$ for some C. The reason for enforcing the second assumption only for $\ell \geqslant \ell_*$ is that for small ℓ, one might have a coincidentally small $S(\ell)$, since it only involves b^ℓ coefficients, while $\check{S}(m)$ is large.

Under this assumption, for $\ell, m \in \mathbb{N}$, $\ell_* \leqslant \ell \leqslant m$, it is possible to bound the sum of the true coefficients, $S(\ell)$, in terms of the observed sum of the discrete coefficients, $\widetilde{S}(\ell, m)$, as follows:

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

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

$$
\begin{aligned}
&\left| \int_{[0,1)^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} - \frac{1}{b^m} \sum_{i=0}^{b^m-1} f(\boldsymbol{x}_i) \right| \\
&\qquad = \left| \hat{f}(\mathbf{0}) - \tilde{f}_m(\mathbf{0}) \right| = \left| \hat{f}_0 - \tilde{f}_{m,0} \right| = \left| \sum_{\lambda=1}^{\infty} \hat{f}_{\lambda b^m} \mathrm{e}^{2\pi\sqrt{-1}\left\langle \tilde{\boldsymbol{k}}(\lambda b^m), \boldsymbol{\Delta}\right\rangle} \right| \\
&\qquad \leqslant \sum_{\lambda=1}^{\infty} \left| \hat{f}_{\lambda b^m} \right| = \widehat{S}(0, m) \leqslant \widehat{\omega}(m) \breve{S}(m) \leqslant \widehat{\omega}(m) \breve{\omega}(m-\ell) S(\ell) \\
&\qquad \leqslant \frac{\widetilde{S}(\ell, m) \widehat{\omega}(m) \breve{\omega}(m-\ell)}{1 - \widehat{\omega}(m-\ell)\breve{\omega}(m-\ell)}.
\end{aligned}
$$

This error bound suggests the following algorithm. Choose $r \in \mathbb{N}$ such that $\widehat{\omega}(r)\breve{\omega}(r) < 1$. For $j \in \mathbb{N}$ define

$$
\ell_j = j + \ell_* - 1, \qquad m_j = j + \ell_* + r - 1, \qquad \mathfrak{C} = \frac{\breve{\omega}(r)}{1 - \widehat{\omega}(r)\breve{\omega}(r)}.
$$

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

$$
\mathfrak{C} \widehat{\omega}(m_j) \widetilde{S}(\ell_j, m_j) \leqslant \varepsilon.
$$

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

Given $\widehat{\omega}$, $\breve{\omega}$, and r, one can compute $\mathfrak{C}$. Alternatively, given $\mathfrak{C}$, $\widehat{\omega}$, and r, one can compute $\breve{\omega}(r)$:

$$
\mathfrak{C} = \frac{\breve{\omega}(r)}{1 - \widehat{\omega}(r)\breve{\omega}(r)} \iff \breve{\omega}(r) = \frac{\mathfrak{C}}{1 + \mathfrak{C}\widehat{\omega}(r)}.
$$

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