

Error Estimation for Cubature Based on Digital Nets

Fred J. Hickernell

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

Abstract

Keywords:

1. Bases and Node Sets

1.1. Group-Like Structures

Consider the half open d -dimensional unit cube, $[0, 1)^d$, on which the functions of interest are to be defined. A commutative additive operation, $\oplus : [0, 1)^d \times [0, 1)^d \rightarrow [0, 1)^d$, is defined by taking digit-by-digit addition modulo some fixed prime number b . Specifically, let $\mathbb{F}_b := \{0, \dots, b-1\}$. For any $x \in [0, 1)$ let \vec{x} denote the sequence of digits of its proper binary expansions, i.e.,

$$\vec{x} = (x_1, x_2, \dots) \in \mathbb{F}_b^\infty \iff x = \sum_{\ell=1}^{\infty} x_\ell b^{-\ell}.$$

Let $\mathbf{x} = (x_1, \dots, x_d)$, and for all $\mathbf{x}, \mathbf{t} \in [0, 1)^d$ define the operations \oplus and \ominus as follows:

$$\begin{aligned} \mathbf{x} &= \left(\sum_{\ell=1}^{\infty} x_{j\ell} b^{-\ell} \right)_{j=1}^d, & \ominus \mathbf{x} &= \left(\sum_{\ell=1}^{\infty} [-x_{j\ell} \bmod b] b^{-\ell} \right)_{j=1}^d, \\ \mathbf{x} \oplus \mathbf{t} &= \left(\sum_{\ell=1}^{\infty} [x_{j\ell} + t_{j\ell} \bmod b] b^{-\ell} \pmod{1} \right)_{j=1}^d. \end{aligned}$$

Here $\mathbf{0}$ is the additive identity. The unique additive inverse of \mathbf{x} is $\ominus \mathbf{x}$, and $\mathbf{x} \ominus \mathbf{t}$ means $\mathbf{x} \oplus (\ominus \mathbf{t})$. Note that under this definition of \oplus ,

$$b\mathbf{x} = \mathbf{0} \quad \forall \mathbf{x} \in [0, 1)^d, \quad \text{where } a\mathbf{x} := \underbrace{\mathbf{x} \oplus \dots \oplus \mathbf{x}}_{a \text{ times}} \quad \forall a \in \mathbb{F}_b.$$

For any given $x \in [0, 1)$ for which \vec{x} does not end in trailing zeros, let t be defined in terms of $\vec{t} = (b-1-x_1, b-1-x_2, \dots)$. Then $t \neq \ominus x$, but $x \oplus t = 0$. Thus,

$$t \oplus (x \oplus (\ominus x)) = t \neq \ominus x = (t \oplus x) \oplus (\ominus x),$$

so we do not have associativity for all of $[0, 1)^d$, and $([0, 1)^d, \oplus)$ is not a group.

Define the following function that determines where an infinite trail of digits $b - 1$ begins when adding two numbers:

$$\text{trail}(\mathbf{x}, \mathbf{t}) = \min_{j=1, \dots, d} \sup\{\ell : (x_{j\ell} + t_{j\ell} \bmod b) \neq b - 1\}. \quad (1a)$$

If one has some $\mathcal{X} \subseteq [0, 1)^d$ for which

$$\text{trail}(\mathbf{x}, \mathbf{t}) = \infty \quad \forall \mathbf{t}, \mathbf{x} \in \mathcal{X}, \quad (1b)$$

then associativity does hold for such \mathcal{X} , i.e.,

$$\mathbf{x} \oplus (\mathbf{t} \oplus \mathbf{u}) = (\mathbf{x} \oplus \mathbf{t}) \oplus \mathbf{u} \quad \forall \mathbf{x}, \mathbf{t}, \mathbf{u} \in \mathcal{X}. \quad (2)$$

If such a subset \mathcal{X} is closed under \oplus , then \mathcal{X} is a commutative group. Moreover, such a set \mathcal{X} is also a vector space under the field \mathbb{F}_b . Note that such a set \mathcal{X} must not have any elements with an infinite trail of any one nonzero digit.

The set \mathbb{N}_0^d is used to index series expressions for the integrands. There exists an Abelian group structure on \mathbb{N}_0^d , with the additive operation \oplus defined as digit-wise addition similarly to the situation of points in the unit cube:

$$\begin{aligned} \vec{k} &= (k_0, k_1, \dots) \in \mathbb{F}_b^\infty \iff k = \sum_{\ell=0}^{\infty} k_\ell b^\ell, \\ \mathbf{k} &= \left(\sum_{\ell=0}^{\infty} k_{j\ell} b^\ell \right)_{j=1}^d, \quad \ominus \mathbf{k} = \left(\sum_{\ell=0}^{\infty} (b - k_{j\ell}) b^\ell \right)_{j=1}^d \quad \forall \mathbf{k} \in \mathbb{N}_0^d, \\ \mathbf{k} \oplus \mathbf{l} &= \left(\sum_{\ell=0}^{\infty} [k_{j\ell} + l_{j\ell} \bmod b] b^\ell \right)_{j=1}^d \quad \forall \mathbf{k}, \mathbf{l} \in \mathbb{N}_0^d. \end{aligned}$$

Since this is a group, we may also define

$$a\mathbf{k} := \underbrace{\mathbf{k} \oplus \dots \oplus \mathbf{k}}_{a \text{ times}} \quad \forall a \in \mathbb{F}_b$$

and note that $b\mathbf{k} = \mathbf{0}$ for all $\mathbf{k} \in \mathbb{N}_0^d$. Moreover, \mathbb{N}_0^d is a vector space over the field \mathbb{F}_b .

Now, define the bilinear operator $\langle \cdot, \cdot \rangle : \mathbb{N}_0^d \times [0, 1)^d \rightarrow \mathbb{F}_b$, where addition and multiplication on \mathbb{F}_b are done modulo b :

$$\langle \mathbf{k}, \mathbf{x} \rangle := \sum_{j=1}^d \sum_{\ell=0}^{\infty} k_{j\ell} x_{j, \ell+1} \pmod{b}. \quad (3a)$$

For all $\mathbf{t}, \mathbf{x} \in [0, 1)^d$, $\mathbf{k}, \mathbf{l} \in \mathbb{N}_0^d$, and $a \in \mathbb{F}_b$, it follows that

$$\langle \mathbf{k}, \mathbf{x} \rangle := \sum_{j=1}^d \sum_{\ell=0}^{\infty} k_{j\ell} x_{j,\ell+1} \pmod{b}, \quad (3b)$$

$$\langle \mathbf{k}, \mathbf{0} \rangle = \langle \mathbf{0}, \mathbf{x} \rangle = 0, \quad (3c)$$

$$\langle \mathbf{k}, a\mathbf{x} \oplus \mathbf{t} \rangle = a \langle \mathbf{k}, \mathbf{x} \rangle + \langle \mathbf{k}, \mathbf{t} \rangle \pmod{b} \quad \text{if } \text{trail}(a\mathbf{x}, \mathbf{t}) = \infty \quad (3d)$$

$$\langle a\mathbf{k} \oplus \mathbf{l}, \mathbf{x} \rangle = a \langle \mathbf{k}, \mathbf{x} \rangle + \langle \mathbf{l}, \mathbf{x} \rangle \pmod{b}, \quad (3e)$$

$$\langle \mathbf{k}, \mathbf{x} \rangle = 0 \quad \forall \mathbf{k} \in \mathbb{N}_0^d \implies \mathbf{x} = \mathbf{0}. \quad (3f)$$

1.2. Sequences, Nets, and Dual Nets

Suppose that there exists a sequence of points in $[0, 1)^d$, denoted $\mathcal{P}_\infty = \{\mathbf{t}_i\}_{i=0}^\infty$ that satisfies (1b) and is closed under \oplus , and so is an abelian group and also a vector space over the field \mathbb{F}_b . Furthermore, \mathcal{P}_∞ is assumed to satisfy the following properties:

$$\{\mathbf{t}_1, \mathbf{t}_b, \mathbf{t}_{b^2}, \dots\} \text{ is linearly independent}, \quad (4a)$$

$$\mathbf{t}_i = \sum_{\ell=0}^{\infty} i_\ell \mathbf{t}_{b^\ell}, \quad \text{where } \vec{i} = (i_0, i_1, i_2, \dots) \in \mathbb{F}_b^\infty, \quad (4b)$$

$$\langle \mathbf{k}, \mathbf{t}_i \rangle = 0 \quad \forall i \in \mathbb{N}_0 \implies \mathbf{k} = \mathbf{0}. \quad (4c)$$

Any $\mathcal{P}_m := \{\mathbf{t}_i\}_{i=0}^{b^m-1}$ is called a *net*. Moreover, \mathcal{P}_m is a subspace of \mathcal{P}_∞ and also a subspace of \mathcal{P}_ℓ for $\ell = m+1, m+2, \dots$, i.e.,

$$\mathcal{P}_0 = \{\mathbf{0}\} \subset \mathcal{P}_1 = \{\mathbf{0}, \mathbf{t}_1, \dots, (b-1)\mathbf{t}_1\} \subset \dots \subset \mathcal{P}_\infty = \{\mathbf{t}_i\}_{i=0}^\infty.$$

We also consider \mathbb{N}_0^d as a vector space with over the field \mathbb{F}_b . For $m \in \mathbb{N}_0$ let $\mathbb{N}_{0,m} := \{0, \dots, b^m - 1\}$, and define the *dual net* corresponding to \mathcal{P}_m as

$$\begin{aligned} \mathcal{P}_m^\perp &= \{\mathbf{k} \in \mathbb{N}_0^d : \langle \mathbf{k}, \mathbf{t}_i \rangle = 0, \quad i = \mathbb{N}_{0,m}\} \\ &= \{\mathbf{k} \in \mathbb{N}_0^d : \langle \mathbf{k}, \mathbf{t}_{b^\ell} \rangle = 0, \quad \ell = 0, \dots, m-1\}. \end{aligned}$$

By this definition $\mathcal{P}_0^\perp = \mathbb{N}_0^d$. The properties of the bilinear transform, (3), implies 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 $\ell = 0, \dots, m-1$, i.e.,

$$\mathcal{P}_0^\perp = \mathbb{N}_0^d \supset \mathcal{P}_1^\perp \supset \dots \supset \mathcal{P}_\infty^\perp = \{\mathbf{0}\}.$$

The next goal is to define a family of maps $\tilde{\nu}_m : \mathbb{N}_0^d \rightarrow \mathbb{N}_{0,m}$ for $m \in \mathbb{N}_0$ that facilitate calculation of the discrete Fourier Walsh transform introduced below.

Definition 1. For every $\mathbf{k} \in \mathbb{N}_0^d$, let

$$\tilde{\nu}_0(\mathbf{k}) := 0, \quad \tilde{\nu}_m(\mathbf{k}) := \sum_{\ell=0}^{m-1} \langle \mathbf{k}, \mathbf{t}_{b^\ell} \rangle b^\ell \in \mathbb{N}_{0,m}, \quad \mathbf{k} \in \mathbb{N}_0^d, \quad m \in \mathbb{N}. \quad (5)$$

Lemma 1. *The following is true for the maps defined in Definition 1. For all $m \in \mathbb{N}_0$ and $\mathbf{k}, \mathbf{l} \in \mathbb{N}_0^d$,*

- a) $\tilde{\nu}_m(\mathbf{0}) = 0$,
- b) *for all $a \in \mathbb{F}_b$ it follows that $\tilde{\nu}_m(a\mathbf{k} \oplus \mathbf{l}) = a\tilde{\nu}_m(\mathbf{k}) \oplus \tilde{\nu}_m(\mathbf{l})$,*
- c) *for all $i \in \mathbb{N}_{0,m}$, $\vec{i} = (i_0, i_1, \dots)$, and $\tilde{\nu}_m(\mathbf{k}) = \nu_0 + \dots + b^{m-1}\nu_{m-1}$, it follows that*

$$\langle \mathbf{k}, \mathbf{t}_i \rangle = \sum_{\ell=0}^{m-1} \nu_\ell i_\ell \pmod{b}, \quad (6)$$

- d) *all $\nu \in \mathbb{N}_{0,m}$ there exists some $\mathbf{r} \in \mathbb{N}_0^d$ with $\tilde{\nu}_m(\mathbf{r}) = \nu$, and*
- e) $\tilde{\nu}_\ell(\mathbf{k}) = \tilde{\nu}_\ell(\mathbf{l}) \forall \ell \in \mathbb{N}_0 \implies \mathbf{k} = \mathbf{l}$.

Proof. Assertion a) follows directly from the definition. Assertion b) follows from Definition 1 and (3e):

$$\begin{aligned} \tilde{\nu}_m(a\mathbf{k} \oplus \mathbf{l}) &= \sum_{\ell=0}^{m-1} \langle a\mathbf{k} \oplus \mathbf{l}, \mathbf{t}_{b^\ell} \rangle b^\ell = \sum_{\ell=0}^{m-1} [a \langle \mathbf{k}, \mathbf{t}_{b^\ell} \rangle + \langle \mathbf{l}, \mathbf{t}_{b^\ell} \rangle \pmod{b}] b^\ell \\ &= \sum_{\ell=0}^{m-1} a \langle \mathbf{k}, \mathbf{t}_{b^\ell} \rangle b^\ell \oplus \sum_{\ell=0}^{m-1} \langle \mathbf{l}, \mathbf{t}_{b^\ell} \rangle b^\ell = a\tilde{\nu}_m(\mathbf{k}) \oplus \tilde{\nu}_m(\mathbf{l}). \end{aligned}$$

Assertion c) follows by applying Definition 1 and (3d):

$$\langle \mathbf{k}, \mathbf{t}_i \rangle = \left\langle \mathbf{k}, \sum_{\ell=0}^{m-1} i_\ell \mathbf{t}_{b^\ell} \right\rangle = \sum_{\ell=0}^{m-1} i_\ell \langle \mathbf{k}, \mathbf{t}_{b^\ell} \rangle \pmod{b} = \sum_{\ell=0}^{m-1} i_\ell \nu_\ell \pmod{b}.$$

To prove assertion d), consider the vector subspace

$$\mathcal{N}_m = \{\boldsymbol{\nu} = (\nu_0, \dots, \nu_{m-1}) \in \mathbb{F}_b^m : \tilde{\nu}(\mathbf{k}) = \nu_0 + \nu_1 b + \dots + \nu_{m-1} b^{m-1} \text{ for some } \mathbf{k} \in \mathbb{N}_0^d\}.$$

Let $\mathbf{i} = (i_0, \dots, i_{m-1}) \in \mathbb{F}_b^m$ be orthogonal with respect to all of the vectors in \mathcal{N}_m . This means that for $i = i_0 + \dots + i_{m-1} b^{m-1} \in \mathbb{N}_{0,m}$, $\langle \mathbf{k}, \mathbf{t}_i \rangle = 0$ for all $\mathbf{k} \in \mathbb{N}_0^d$ by (6). Then by (4c) it follows that $\mathbf{i} = \mathbf{0}$. Since this is the only vector that is perpendicular to \mathcal{N}_m , we must have $\mathcal{N}_m = \mathbb{F}_b^m$, which proves d).

To prove e) suppose that $\tilde{\nu}_\ell(\mathbf{k}) = \tilde{\nu}_\ell(\mathbf{l})$ for all $\ell \in \mathbb{N}_0$. It follows from c) that

$$\langle \mathbf{k} \ominus \mathbf{l}, \mathbf{t}_\ell \rangle = \langle \mathbf{k}, \mathbf{t}_\ell \rangle - \langle \mathbf{l}, \mathbf{t}_\ell \rangle \pmod{b} = 0 \quad \forall \ell \in \mathbb{N}_0.$$

By (4c) one must have $\mathbf{k} \ominus \mathbf{l} = \mathbf{0}$, which implies that $\mathbf{k} = \mathbf{l}$. \square

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 $\{\varphi(\cdot, \mathbf{k}) \in \mathcal{L}_2([0, 1]^d) : \mathbf{k} \in \mathbb{N}_0^d\}$ be the complete orthonormal Walsh function *basis* for $\mathcal{L}_2([0, 1]^d)$, i.e.,

$$\varphi(\mathbf{x}, \mathbf{k}) = e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x} \rangle / b}, \quad \mathbf{k} \in \mathbb{N}_0^d, \quad \mathbf{x} \in [0, 1]^d.$$

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

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) \varphi(\mathbf{x}, \mathbf{k}), \quad \text{where } \hat{f}(\mathbf{k}) = \langle f, \varphi(\cdot, \mathbf{k}) \rangle_2, \quad (7)$$

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

$$\langle f, g \rangle_2 = \sum_{\mathbf{k} \in \mathbb{N}_0^d} \hat{f}(\mathbf{k}) \overline{\hat{g}(\mathbf{k})} =: \left\langle (\hat{f}(\mathbf{k}))_{\mathbf{k} \in \mathbb{N}_0^d}, (\hat{g}(\mathbf{k}))_{\mathbf{k} \in \mathbb{N}_0^d} \right\rangle_2.$$

For all $\mathbf{k} \in \mathbb{N}_0^d$ and $\mathbf{x} \in \mathcal{P}$, it follows that

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

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.

$$\frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{t}_i \rangle} = \mathbb{1}_{\mathcal{P}_m^\perp}(\mathbf{k}) = \begin{cases} 1, & \mathbf{k} \in \mathcal{P}_m^\perp \\ 0, & \mathbf{k} \in \mathbb{N}_0^d \setminus \mathcal{P}_m^\perp. \end{cases}$$

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

$$\begin{aligned}
\tilde{f}_m(\mathbf{k}) &:= \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_i \rangle / b} f(\mathbf{x}_i) \\
&= \frac{1}{b^m} \sum_{i=0}^{b^m-1} \left[e^{-2\pi\sqrt{-1}\langle \mathbf{k}, \mathbf{x}_i \rangle / b} \sum_{\mathbf{l} \in \mathbb{N}_0^d} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l}, \mathbf{x}_i \rangle / b} \right] \\
&= \sum_{\mathbf{l} \in \mathbb{N}_0^d} \hat{f}(\mathbf{l}) \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \mathbf{x}_i \rangle / b} \\
&= \sum_{\mathbf{l} \in \mathbb{N}_0^d} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \Delta \rangle / b} \frac{1}{b^m} \sum_{i=0}^{b^m-1} e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \mathbf{t}_i \rangle / b} \\
&= \sum_{\mathbf{l} \in \mathbb{N}_0^d} \hat{f}(\mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l} \ominus \mathbf{k}, \Delta \rangle / b} \mathbb{1}_{\mathcal{P}_m^\perp}(\mathbf{l} \ominus \mathbf{k}) \\
&= \sum_{\mathbf{l} \in \mathcal{P}_m^\perp} \hat{f}(\mathbf{k} \oplus \mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l}, \Delta \rangle / b} \\
&= \hat{f}(\mathbf{k}) + \sum_{\mathbf{l} \in \mathcal{P}_m^\perp \setminus \mathbf{0}} \hat{f}(\mathbf{k} \oplus \mathbf{l}) e^{2\pi\sqrt{-1}\langle \mathbf{l}, \Delta \rangle / b}, \quad \forall \mathbf{k} \in \mathbb{N}_0^d. \tag{9}
\end{aligned}$$

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 (7), 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 (8) 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 $\mathbf{k} \in \mathbb{N}_0^d$ 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

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

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 $\tilde{\mathbf{k}}(\kappa) \in \mathbb{N}_0^d$ 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 $m \in \mathbb{N}$:

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

where $\mathring{f}_{m,\kappa} := \mathring{f}_m(\tilde{\nu}_m(\tilde{\mathbf{k}}(\kappa)))$. According to (9), it follows that

$$\tilde{f}_{m,\kappa} = \hat{f}_\kappa + \sum_{\lambda=1}^{\infty} \hat{f}_{\kappa+\lambda b^m} e^{2\pi\sqrt{-1}\langle \tilde{\mathbf{k}}(\kappa+\lambda b^m) \ominus \tilde{\mathbf{k}}(\kappa), \mathbf{\Delta} \rangle / b}. \quad (10)$$

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 $\ell, m \in \mathbb{N}_0$, $\ell \leq m$:

$$\begin{aligned} S(m) &= \sum_{\kappa=\lfloor b^{m-1} \rfloor}^{b^m-1} |\hat{f}_\kappa|, & \hat{S}(\ell, m) &= \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} \sum_{\lambda=1}^{\infty} |\hat{f}_{\kappa+\lambda b^m}|, \\ \check{S}(m) &= \hat{S}(0, m) + \cdots + \hat{S}(m, m) = \sum_{\kappa=b^m}^{\infty} |\hat{f}_\kappa|, \\ \check{S}(\ell, m) &= \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} |\tilde{f}_{m,\kappa}| = \sum_{\kappa=\lfloor b^{\ell-1} \rfloor}^{b^\ell-1} |\mathring{f}_{m,\kappa}|. \end{aligned}$$

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

We now make critical assumptions that $\hat{S}(\ell, m)$ 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 $\ell \leq m$, and fix $\ell_* \in \mathbb{N}$. It is assumed that there exist known, non-negative valued functions $\hat{\omega}$ and $\check{\omega}$ with $\lim_{m \rightarrow \infty} \check{\omega}(m) = 0$ such that

$$\hat{S}(\ell, m) \leq \hat{\omega}(m - \ell) \check{S}(m) \quad \forall \ell, \quad \check{S}(m) \leq \check{\omega}(m - \ell) S(\ell) \quad \forall \ell_* \leq \ell. \quad (11)$$

By the definition of $\check{S}(m)$, the choice $\hat{\omega}(m) := 1$ for all m is always guaranteed to work. However, one might also consider choosing $\hat{\omega}(m) = Cb^{-m}$ for some C . The reason for enforcing the second assumption only for $\ell \geq \ell_*$ 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 $\ell, m \in \mathbb{N}$, $\ell_* \leq \ell \leq m$, it is possible to bound the sum of the true coefficients, $S(\ell)$, in terms of the observed sum of the discrete

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

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

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

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

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

$$\ell_j = j + \ell_* - 1, \quad m_j = j + \ell_* + r - 1, \quad \mathfrak{C} = \frac{\check{\omega}(r)}{1 - \hat{\omega}(r) \check{\omega}(r)}.$$

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

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

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

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

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