Error Estimation for Cubature Based on Digital Nets

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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, $\oplus : [0,1)^d \times [0,1)^d \to [0,1)^d$, is defined by taking digit-by-digit addition modulo some fixed prime number b. Specifically, let $\mathbb{F}_b := \{0,\ldots,b-1\}$. For any $x \in [0,1)$ let $\vec{x}$ denote the sequence of digits of its proper binary expansions, i.e.,

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

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

$$\boldsymbol{x} = \left(\sum_{\ell=1}^{\infty} x_{j\ell} b^{-\ell}\right)_{j=1}^{d}, \qquad \ominus\boldsymbol{x} = \left(\sum_{\ell=1}^{\infty} [-x_{j\ell} \bmod b] b^{-\ell}\right)_{j=1}^{d},$$

$$\boldsymbol{x} \oplus \boldsymbol{t} = \left(\sum_{\ell=1}^{\infty} [x_{j\ell} + t_{j\ell} \bmod b] b^{-\ell} \pmod 1\right)_{j=1}^{d}.$$

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

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

For any given $x \in [0,1)$ for which $\vec{x}$ does not end in trailing zeros, let t be defined in terms of $\vec{t} = (b-1-x_1, b-1-x_2, \ldots)$. 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:

$$\operatorname{trail}(\boldsymbol{x}, \boldsymbol{t}) = \min_{j=1,\ldots,d} \sup\{\ell : (x_{j\ell} + t_{j\ell} \bmod b) \neq b-1\}. \tag{1a}$$

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

$$\operatorname{trail}(\boldsymbol{x}, \boldsymbol{t}) = \infty \qquad \forall \boldsymbol{t}, \boldsymbol{x} \in \mathcal{X}, \tag{1b}$$

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

$$\boldsymbol{x} \oplus (\boldsymbol{t} \oplus \boldsymbol{u}) = (\boldsymbol{x} \oplus \boldsymbol{t}) \oplus \boldsymbol{u} \qquad \forall \boldsymbol{x}, \boldsymbol{t}, \boldsymbol{u} \in \mathcal{X}. \tag{2}$$

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:

$$\vec{k} = (k_0, k_1, \ldots) \in \mathbb{F}_b^\infty \Longleftrightarrow k = \sum_{\ell=0}^{\infty} k_\ell b^\ell,$$

$$\boldsymbol{k} = \left(\sum_{\ell=0}^{\infty} k_{j\ell} b^\ell\right)_{j=1}^d, \qquad \ominus \boldsymbol{k} = \left(\sum_{\ell=0}^{\infty} (b - k_{j\ell}) b^\ell\right)_{j=1}^d \qquad \forall \boldsymbol{k} \in \mathbb{N}_0^d,$$

$$\boldsymbol{k} \oplus \boldsymbol{l} = \left(\sum_{\ell=0}^{\infty} [k_{j\ell} + l_{j\ell} \bmod b] b^\ell\right)_{j=1}^d \qquad \forall \boldsymbol{k}, \boldsymbol{l} \in \mathbb{N}_0^d.$$

Since this is a group, we may also define

$$a\boldsymbol{k} := \underbrace{\boldsymbol{k} \oplus \cdots \oplus \boldsymbol{k}}_{a \text{ times}} \ \forall a \in \mathbb{F}_b$$

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

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

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

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

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

$$\langle \boldsymbol{k}, \boldsymbol{0} \rangle = \langle \boldsymbol{0}, \boldsymbol{x} \rangle = 0, \tag{3c}$$

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

$$\langle a\boldsymbol{k} \oplus \boldsymbol{l}, \boldsymbol{x} \rangle = a \langle \boldsymbol{k}, \boldsymbol{x} \rangle + \langle \boldsymbol{l}, \boldsymbol{x} \rangle \pmod b, \tag{3e}$$

$$\langle \boldsymbol{k}, \boldsymbol{x} \rangle = 0 \ \forall \boldsymbol{k} \in \mathbb{N}_0^d \implies \boldsymbol{x} = \boldsymbol{0}. \tag{3f}$$

1.2. Sequences, Nets, and Dual Nets

Suppose that there exists a sequence of points in $[0,1)^d$, denoted $\mathcal{P}_\infty = \{\boldsymbol{t}_i\}_{i=0}^{\infty}$ 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, $\mathcal{P}_\infty$ is assumed to satisfy the following properties:

$$\{\boldsymbol{t}_1, \boldsymbol{t}_b, \boldsymbol{t}_{b^2}, \ldots\} \text{ is linearly independent}, \tag{4a}$$

$$\boldsymbol{t}_i = \sum_{\ell=0}^{\infty} i_\ell \boldsymbol{t}_{b^\ell}, \qquad \text{where } \vec{\imath} = (i_0, i_1, i_2, \ldots) \in \mathbb{F}_b^\infty, \tag{4b}$$

$$\langle \boldsymbol{k}, \boldsymbol{t}_i \rangle = 0 \ \forall i \in \mathbb{N}_0 \implies \boldsymbol{k} = \boldsymbol{0}. \tag{4c}$$

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

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

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 $\mathbb{N}_{0,m} := \{0, \ldots, b^m - 1\}$, and define the *dual net* corresponding to $\mathcal{P}_m$ as

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

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

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

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

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

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

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

a) $\tilde{\nu}_m(\mathbf{0}) = 0$*,*
b) *for all* $a \in \mathbb{F}_b$ *it follows that* $\tilde{\nu}_m(a\boldsymbol{k} \oplus \boldsymbol{l}) = a\tilde{\nu}_m(\boldsymbol{k}) \oplus \tilde{\nu}_m(\boldsymbol{l})$*,*
c) *for all* $i \in \mathbb{N}_{0,m}$*,* $\vec{\imath} = (i_0, i_1, \ldots)$*, and* $\tilde{\nu}_m(\boldsymbol{k}) = \nu_0 + \cdots + b^{m-1}\nu_{m-1}$*, it follows that*
$$\langle \boldsymbol{k}, \boldsymbol{t}_i \rangle = \sum_{\ell=0}^{m-1} \nu_\ell i_\ell \pmod b, \tag{6}$$
d) *all* $\nu \in \mathbb{N}_{0,m}$ *there exists some* $\boldsymbol{r} \in \mathbb{N}_0^d$ *with* $\tilde{\nu}_m(\boldsymbol{r}) = \nu$*, and*
e) $\tilde{\nu}_\ell(\boldsymbol{k}) = \tilde{\nu}_\ell(\boldsymbol{l})\, \forall \ell \in \mathbb{N}_0 \Longrightarrow \boldsymbol{k} = \boldsymbol{l}$*.*

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

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

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

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

To prove assertion d), consider the vector subspace

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

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

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

$$
\begin{aligned}
\tilde{f}_m(\boldsymbol{k}) &:= \frac{1}{b^m}\sum_{i=0}^{b^m-1} \mathrm{e}^{-2\pi\sqrt{-1}\langle \boldsymbol{k},\boldsymbol{x}_i\rangle/b} f(\boldsymbol{x}_i) \qquad (8)\\
&= \frac{1}{b^m}\sum_{i=0}^{b^m-1} \left[\mathrm{e}^{-2\pi\sqrt{-1}\langle \boldsymbol{k},\boldsymbol{x}_i\rangle/b} \sum_{\boldsymbol{l}\in\mathbb{N}_0^d} \hat{f}(\boldsymbol{l})\mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l},\boldsymbol{x}_i\rangle/b}\right]\\
&= \sum_{\boldsymbol{l}\in\mathbb{N}_0^d} \hat{f}(\boldsymbol{l}) \frac{1}{b^m}\sum_{i=0}^{b^m-1} \mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}\ominus\boldsymbol{k},\boldsymbol{x}_i\rangle/b}\\
&= \sum_{\boldsymbol{l}\in\mathbb{N}_0^d} \hat{f}(\boldsymbol{l}) \mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}\ominus\boldsymbol{k},\boldsymbol{\Delta}\rangle/b} \frac{1}{b^m}\sum_{i=0}^{b^m-1} \mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}\ominus\boldsymbol{k},\boldsymbol{t}_i\rangle/b}\\
&= \sum_{\boldsymbol{l}\in\mathbb{N}_0^d} \hat{f}(\boldsymbol{l}) \mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l}\ominus\boldsymbol{k},\boldsymbol{\Delta}\rangle/b} \mathbb{1}_{\mathcal{P}_m^\perp}(\boldsymbol{l}\ominus\boldsymbol{k})\\
&= \sum_{\boldsymbol{l}\in\mathcal{P}_m^\perp} \hat{f}(\boldsymbol{k}\oplus\boldsymbol{l}) \mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l},\boldsymbol{\Delta}\rangle/b}\\
&= \hat{f}(\boldsymbol{k}) + \sum_{\boldsymbol{l}\in\mathcal{P}_m^\perp\backslash\boldsymbol{0}} \hat{f}(\boldsymbol{k}\oplus\boldsymbol{l}) \mathrm{e}^{2\pi\sqrt{-1}\langle \boldsymbol{l},\boldsymbol{\Delta}\rangle/b}, \qquad \forall \boldsymbol{k}\in\mathbb{N}_0^d. \qquad (9)
\end{aligned}
$$

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 (7), plus the *aliasing* terms corresponding to $\hat{f}(\boldsymbol{l})$ where $\boldsymbol{l}\ominus\boldsymbol{k}\in\mathcal{P}_m^\perp\backslash\boldsymbol{0}$.

1.4. Computation of the Discrete Transform

The discrete transform defined in (8) may also be expressed as

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

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 $\boldsymbol{k} \in \mathbb{N}_0^d$ with $\tilde{\nu}_m(\boldsymbol{k}) = \nu = \nu_0 + \nu_1 b + \cdots + \nu_{m-1} b^{m-1}$ one may write

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

This sum can be computed recursively:

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

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

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

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 $\tilde{\boldsymbol{k}}(\kappa) \in \mathbb{N}_0^d$ 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 $\tilde{\boldsymbol{k}}(\kappa) \ominus \tilde{\boldsymbol{k}}(\kappa + \lambda b^m) \in \mathcal{P}_m^\perp$.

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

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

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

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

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

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

The first three kinds of sums, $S(\cdot)$, $\widehat{S}(\cdot,\cdot)$, and $\breve{S}(\cdot)$, 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 $\breve{S}(m)$ 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 $\breve{\omega}$ with $\lim_{m\to\infty} \breve{\omega}(m) = 0$ such that

$$\widehat{S}(\ell, m) \leqslant \widehat{\omega}(m-\ell)\breve{S}(m) \quad \forall \ell, \qquad \breve{S}(m) \leqslant \breve{\omega}(m-\ell)S(\ell) \quad \forall \ell_* \leqslant \ell. \tag{11}$$

By the definition of $\breve{S}(m)$, 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 $\breve{S}(m)$ 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

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

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 $\breve{\omega}(r)$:

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