Variance-based sensitivity analysis using harmonic analysis

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Abstract

Fourier Amplitude Sensitivity Test (FAST) and Random Balance Design (RBD) are popular methods of estimating variance-based sensitivity indices. We revisit them in light of the discrete Fourier transform (DFT) on finite subgroups of the torus and randomized orthogonal array sampling. We then study the estimation error of both these methods. This allows to improve FAST and to derive explicit rates of convergence of its estimators by using the framework of lattice rules. We also give a natural generalization of the classic RBD by using randomized orthogonal arrays having any parameters, and we provide a bias correction method for its estimators.

Keywords: global sensitivity analysis, random balance design, Fourier amplitude sensitivity test, orthogonal arrays, lattice rules

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1 Introduction

Variance-based sensitivity analysis consists in computing indices — the so-called variance-based sensitivity indices (SI) or Sobol' indices (see [34]) — that are essentially multiple integrals. Many numerical techniques have been developed to estimate these quantities. This includes the crude Monte Carlo estimator (see [34], and [18] for a recent work), the polynomial chaos-based estimators (see [37] and [2]) and the FAST method (see [9] and [30]) as well as its derived approach, RBD (see [38]), and their hybrid approach, RBD-FAST (see [38] and [24]), and many others (see [29] for a review).

The main purpose of this paper is to revisit FAST and RBD by using the discrete harmonic analysis framework, in order to carry out a theoretical error analysis. In these methods the SI estimation amounts to computing a finite number of the complex Fourier coefficients of the model of interest defined on the unit hypercube. In theory these computations could be done by performing a crude Monte Carlo integration or a cubature on a regular grid. But the rate of convergence of the Monte Carlo method is low, and cubatures are generally unfeasible in high dimension because of the exponential growth of the number of nodes, also known as the curse of dimensionality.

A first possible starting point to overcome these drawbacks is to note that the discrete complex Fourier coefficients computed by using the cubature approach are exactly the coefficients in the representation of the trigonometric interpolation polynomial of the model of interest on the regular grid. Consequently this approach consists of a trigonometric interpolation issue and can be generalized by using Smolyak algorithm on sparse grids (see [12]). Such interpolation schemes are quite efficient as long as the model of interest is sufficiently smooth (see [3]). But the matrix of the interpolation operator in such a method suffers from an increase of its condition number for both increasing refinement of the regular grid and increasing model dimension, and thus makes the interpolation scheme unstable (see [19]).

As a consequence, it turns out to be obvious that, in order to avoid the stability issue, one has to focus on unitary operators. Thus DFT operators on finite subgroups of the torus (see e.g. [23]) — i.e. the unit hypercube view as a group — whose matrices have a perfect condition number equal to 1 are particularly well-suited in the present framework. This leads to the use of lattice rules (see [33] for a review) to which FAST, as shown in Subsection 4.1, is closely related. In a second time, by viewing finite subgroups of the torus as orthogonal arrays (see [16] for a review), the previous method can be generalized by performing a randomization process on these arrays. This leads to the use of randomized orthogonal arrays in numerical integration (see [26] and references therein) to which RBD, as shown in Subsection 4.2, is closely related.

The paper proceeds as follows. In Section 2, we set up the notation, we give background materials related to the ANOVA decomposition and to the Fourier series representation, and we introduce the class of estimators of interest. In Section 3, we first review both FAST and RBD, and then revisit them. Section 4 is devoted to the error analysis by using the revisited definition provided in Section 3. At last, Section 5 gives numerical illustrations of RBD estimates on an analytical model. Most of the proofs of the propositions are given in appendix A.

2 Background

2.1 Notation

First, $\mathbb{E}[Y]$, $\mathbb{E}[Y|X]$ and $\mathrm{Var}[Y]$ denote the unconditional expectation of Y, the conditional expectation of Y given X and the variance of Y, respectively. By convention, we define $\mathbb{E}[Y|\emptyset] = \mathbb{E}[Y]$. Secondly, consider a parameter d in $\mathbb{N}^*$ — the dependence on which is omitted for convenience — and define for any $\mathfrak{u} \in \{1, \dots, d\}$,

$$\begin{aligned}\mathbb{Z}_{\mathfrak{u}} &= \{\mathbf{k} \in \mathbb{Z}^d \mid \forall i \in \mathfrak{u},\ k_i \in \mathbb{Z} \text{ and } \forall i \notin \mathfrak{u},\ k_i = 0\} \\ \mathbb{Z}^*_{\mathfrak{u}} &= \{\mathbf{k} \in \mathbb{Z}^d \mid \forall i \in \mathfrak{u},\ k_i \in \mathbb{Z}^* \text{ and } \forall i \notin \mathfrak{u},\ k_i = 0\}\end{aligned}$$

and for all $i \in \mathbb{N}^*$,

$$\begin{aligned}\mathbb{Z}_{\mathfrak{u}}(i) &= \mathbb{Z}_{\mathfrak{u}} \cap \Big(-\frac{i}{2}, \frac{i}{2}\Big]^d \\ \mathbb{Z}^*_{\mathfrak{u}}(i) &= \mathbb{Z}^*_{\mathfrak{u}} \cap \Big(-\frac{i}{2}, \frac{i}{2}\Big]^d.\end{aligned}$$

Lastly, a design of experiments is commonly denoted by D and, for $i \in \mathbb{N}^*$, the notation $D(i)$ refers to the regular grid in $[0,1)^d$

$$D(i) = \left\{0, \frac{1}{i}, \dots, \frac{i-1}{i}\right\}^d .$$

2.2 Variance-based sensitivity indices

Let $\mathbf{X} = (X_1, \dots, X_d) \in [0,1]^d$ be a d-dimensional random vector and let us consider $Y = f(\mathbf{X})$ where $f : [0,1]^d \to \mathbb{R}$ is a measurable function such that $\mathbb{E}[Y^2] < +\infty$. Under the assumption that

$\mathbf{X}$ has independent components, the Hoeffding decomposition [17, 41] states that Y can be uniquely decomposed into summands of increasing dimensions

$$Y - \mathbb{E}[Y] = \sum_{m=1}^{d} \sum_{\substack{\mathfrak{u} \subseteq \{1,\ldots,d\} \\ |\mathfrak{u}|=m}} f_{\mathfrak{u}}(X_i, i \in \mathfrak{u}) \tag{1}$$

where the $2^d - 1$ random variables on the right-hand side of (1) should satisfy the property

$$\forall \mathfrak{v} \subsetneq \mathfrak{u}, \quad \mathbb{E}\big[f_{\mathfrak{u}}(X_i, i \in \mathfrak{u}) | X_i, i \in \mathfrak{v}\big] = 0 \ . \tag{2}$$

Note that in this case the random variables $f_{\mathfrak{u}}(X_i, i \in \mathfrak{u})$ have mean zero and are mutually uncorrelated. Therefore taking the variance of both sides in (1) gives the variance decomposition [14, 34] of Y

$$\mathrm{Var}[Y] = \sum_{m=1}^{d} \sum_{\substack{\mathfrak{u} \subseteq \{1,\ldots,d\} \\ |\mathfrak{u}|=m}} \mathrm{Var}\big[f_{\mathfrak{u}}(X_i, i \in \mathfrak{u})\big].$$

Finally, if $\mathrm{Var}[Y] \neq 0$, we define the so-called variance-based sensitivity indices — or Sobol' indices — as

$$\mathrm{S}_{\mathfrak{u}}(f, \mathbf{X}) = \frac{\mathrm{Var}\big[f_{\mathfrak{u}}(X_i, i \in \mathfrak{u})\big]}{\mathrm{Var}[Y]} \ .$$

In practice, global sensitivity analysis focuses on computing the first-order ($|\mathfrak{u}| = 1$) and the second-order ($|\mathfrak{u}| = 2$) terms.

2.3 Fourier series representation

From here on let us assume that the X_i's are independent and uniformly distributed on $[0, 1]$. Therefore the joint probability density function of $\mathbf{X}$ on $[0, 1]^d$ is equal to 1 and, denoting

$$P_{\mathbf{n}}(f, \mathbf{X}) = \sum_{k_1=-n_1}^{n_1} \cdots \sum_{k_d=-n_d}^{n_d} \mathrm{c}_{\mathbf{k}}(f) \exp(2i\pi \mathbf{k} \cdot \mathbf{X})$$

where

$$\mathrm{c}_{\mathbf{k}}(f) = \int_{[0,1]^d} f(\mathbf{X}) \exp(-2i\pi \mathbf{k} \cdot \mathbf{X}) d\mathbf{X} \ ,$$

the Riesz-Fischer theorem yields

$$P_{\mathbf{n}}(f, \mathbf{X}) \ \xrightarrow{L^2} \ Y \ .$$

In particular, we have

$$Y = \sum_{k_1 \in \mathbb{Z}} \cdots \sum_{k_d \in \mathbb{Z}} \mathrm{c}_{\mathbf{k}}(f) \exp(2i\pi \mathbf{k} \cdot \mathbf{X}) \quad \text{a. s.} \tag{3}$$

and as the following proposition shows, this Fourier series representation gives an harmonic approach to handle the variance-based sensitivity indices.

Proposition 1. *Let $X_1, \ldots, X_d$ be independent random variables uniformly distributed on $[0,1]$ and let us consider $Y = f(\mathbf{X})$ where $f : [0,1]^d \to \mathbb{R}$ is a measurable function such that $\mathbb{E}[Y^2] < +\infty$ and $\mathrm{Var}[Y] \neq 0$. Then for any non-empty subset $\mathfrak{u}$ of $\{1, \ldots, d\}$ we have*

$$\mathrm{S}_{\mathfrak{u}}(f, \mathbf{X}) = \frac{\sum_{\mathbf{k} \in \mathbb{Z}_{\mathfrak{u}}^*} \left|\mathrm{c}_{\mathbf{k}}(f)\right|^2}{\sum_{\mathbf{k} \in (\mathbb{Z}^d)^*} \left|\mathrm{c}_{\mathbf{k}}(f)\right|^2} . \tag{4}$$

Proof. In view of (3), it is easy to notice that the components in the Hoeffding decomposition satisfy

$$f_{\mathfrak{u}}(X_i, i \in \mathfrak{u}) = \sum_{\mathbf{k} \in \mathbb{Z}_{\mathfrak{u}}^*} \mathrm{c}_{\mathbf{k}}(f) \exp(2i\pi \mathbf{k} \cdot \mathbf{X}) \quad \text{a. s.}$$

and the conclusion follows from Parseval's identity. □

As in (4) the index $\mathrm{S}_{\mathfrak{u}}(f, \mathbf{X})$ does no more depend on $\mathbf{X}$ we now simply denote the sensitivity indices by $\mathrm{S}_{\mathfrak{u}}(f)$. In the same way, we now denote $\mathrm{V}_{\mathfrak{u}}(f)$ and $\mathrm{V}(f)$ the parts of variance $\mathrm{Var}\left[f_{\mathfrak{u}}(X_i, i \in \mathfrak{u})\right]$ and the total variance $\mathrm{Var}[Y]$, respectively. Lastly, when $\mathfrak{u} = \{i_1, \ldots, i_s\}$ is explicitely given, we use the more common notation $\mathrm{V}_{i_1 \ldots i_s}(f)$ and $\mathrm{S}_{i_1 \ldots i_s}(f)$.

2.4 Estimation

We now define basic estimators based on Proposition 1. For any non-empty subset $\mathfrak{u}$ of $\{1, \ldots, d\}$, let $K_{\mathfrak{u}}$ be a finite subset of $\mathbb{Z}_{\mathfrak{u}}^*$ and D a finite subset of $[0,1)^d$ with $|D| = n$. Denoting

$$\widehat{\mathrm{c}}_{\mathbf{k}}(f, D) = \frac{1}{n} \sum_{\mathbf{x} \in D} f(\mathbf{x}) \exp(-2i\pi \mathbf{k} \cdot \mathbf{x}), \tag{5}$$

we define the estimator of $\mathrm{V}_{\mathfrak{u}}(f)$ as the truncated series

$$\widehat{\mathrm{V}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, D) = \sum_{\mathbf{k} \in K_{\mathfrak{u}}} \left|\widehat{\mathrm{c}}_{\mathbf{k}}(f, D)\right|^2 , \tag{6}$$

the estimator of $\mathrm{V}(f)$ as the empirical variance

$$\widehat{\mathrm{V}}(f, D) = \frac{1}{n} \sum_{\mathbf{x} \in D} \Big(f(\mathbf{x}) - \frac{1}{n} \sum_{\mathbf{y} \in D} f(\mathbf{y}) \Big)^2 \tag{7}$$

and the estimator of $\mathrm{S}_{\mathfrak{u}}(f)$ naturally as

$$\widehat{\mathrm{S}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, D) = \frac{\widehat{\mathrm{V}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, D)}{\widehat{\mathrm{V}}(f, D)}. \tag{8}$$

Example 1. *If the design of experiments D is a set of independent random points uniformly distributed on $[0,1]^d$ and*

$$K = \bigsqcup_{\substack{\mathfrak{u} \subseteq \{1,\dots,d\} \\ \mathfrak{u} \neq \emptyset}} K_{\mathfrak{u}},$$

we have

$$\widehat{\mathrm{V}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, D) = \mathrm{V}_{\mathfrak{u}}(\tilde{f})$$

where

$$\tilde{f}(\mathbf{X}) = \sum_{\mathbf{k} \in K \cup \{\mathbf{0}\}} \widehat{\mathrm{c}}_{\mathbf{k}}(f, D) \mathrm{e}^{2i\pi \mathbf{k}\cdot\mathbf{X}}$$

is the approximation of $f(\mathbf{X})$ using the quasi-regression approach [1] *based on the random sample D. Note that $|\widehat{\mathrm{c}}_{\mathbf{k}}(f,D)|^2$ is a biased estimator of $|\mathrm{c}_{\mathbf{k}}(f,D)|^2$ and it is recommended to use the unbiased estimator*

$$\frac{n}{n-1}\left(|\widehat{\mathrm{c}}_{\mathbf{k}}(f,D)|^2 - \frac{1}{n^2}\sum_{\mathbf{x} \in D} f^2(\mathbf{x})\right)$$

(see e.g. [22]*). In the same way, the empirical variance $\widehat{\mathrm{V}}(f,D)$ should be replaced by the unbiased sample variance $\frac{n}{n-1}\widehat{\mathrm{V}}(f,D)$.*

Example 2. *If the design of experiments D is the regular grid $D(q)$ — with $n = q^d$, $q \in \mathbb{N}^*$ — and if for all non-empty subsets $\mathfrak{u}$ of $\{1,\dots,d\}$, $K_{\mathfrak{u}} = \mathbb{Z}^*_{\mathfrak{u}}(q)$ and*

$$K = \bigsqcup_{\substack{\mathfrak{u} \subseteq \{1,\dots,d\} \\ \mathfrak{u} \neq \emptyset}} K_{\mathfrak{u}}$$

then by Parseval's identity, it can be easily shown that

$$\widehat{\mathrm{S}}_{\mathfrak{u}}\big(f, K_{\mathfrak{u}}, D(q)\big) = \mathrm{S}_{\mathfrak{u}}(\tilde{f})$$

where

$$\tilde{f}(\mathbf{x}) = \sum_{\mathbf{k} \in K} \widehat{\mathrm{c}}_{\mathbf{k}}\big(f, D(q)\big) \mathrm{e}^{2i\pi \mathbf{k}\cdot\mathbf{x}}$$

is the trigonometric interpolation polynomial of $f(\mathbf{x})$ (see e.g. [11]*) at the $n = q^d$ equally spaced nodes $\mathbf{x} \in D(q)$.*

3 New introduction to FAST and RBD

In the sequel, since the X_i's are independent and uniformly distributed on $[0,1]$, we have

$$\mathbb{E}\big[f(\mathbf{X})\big] = \int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x}$$

so we use no more probabilistic notation. Moreover, the integrability assumption on f now reads $f \in L^2([0,1]^d)$.

3.1 Review of FAST

3.1.1 Numerical integration

FAST is essentially an application of the following result due to Weyl [43] (see also the Weyl's ergodic theorem [42] in german or [32])

Theorem 1. [Weyl] *Let g be a bounded Riemann integrable function on $[0,1]^d$ and for all $i = 1,\dots,d$, $x_i(t) = \{\omega_i t\}$ where the ω_i's are real numbers linearly independent over $\mathbb{Q}$ and $\{\cdot\}$ denotes the fractional part, then*

$$\int_{[0,1]^d} g(\mathbf{x})d\mathbf{x} = \lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} g\big(x_1(t),\dots,x_d(t)\big)dt. \tag{9}$$

In particular, for any $\mathbf{k} \in \mathbb{Z}^d$ and $g : \mathbf{x} \mapsto f(\mathbf{x})\exp\big(-2i\pi\mathbf{k}\cdot\mathbf{x}\big)$, (9) reads

$$\mathrm{c}_{\mathbf{k}}(f) = \lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} f\circ\mathbf{x}(t)\exp\big(-2i\pi(\mathbf{k}\cdot\boldsymbol{\omega})t\big)dt. \tag{10}$$

Then FAST consists in replacing $x_i(t) = \{\omega_i t\}$ with semiparametric functions $x_i(t) = G_i\big(\sin(\omega_i t)\big)$ (see [8]) where the ω_i's are positive integers and the transformations G_i are chosen to preserve the marginal distributions of the X_i's. If the latter are uniformly distributed — as in the present paper —, it can be shown (see [9] and [30]) that $G_i(\cdot) = \frac{1}{\pi}\arcsin(\cdot) + \frac{1}{2}$. Saltelli et al. [30] also propose to add a random phase-shift $\varphi_i \in [0,2\pi)$, getting the semiparametric functions $x_i^*(t) = \frac{1}{\pi}\arcsin\big(\sin(2\pi\omega_i t + \varphi_i)\big) + \frac{1}{2}$. Hence, replacing $\mathbf{x}$ with $\mathbf{x}^*$ in (10) gives

$$\mathrm{c}_{\mathbf{k}}(f) \approx \lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} f\circ\mathbf{x}^*(t)\exp\big(-2i\pi(\mathbf{k}\cdot\boldsymbol{\omega})t\big)dt.$$

Thus, since the functions x_i^* are 1-periodic, it comes

$$\mathrm{c}_{\mathbf{k}}(f) \approx \int_0^1 f\circ\mathbf{x}^*(t)\exp\big(-2i\pi(\mathbf{k}\cdot\boldsymbol{\omega})t\big)dt$$

and applying the rectangle rule to the right-hand side integral gives

$$\mathrm{c}_{\mathbf{k}}(f) \approx \widehat{\mathrm{c}}_{\mathbf{k}\cdot\boldsymbol{\omega}}(f\circ\mathbf{x}^*). \tag{11}$$

where

$$\widehat{\mathrm{c}}_{\mathbf{k}\cdot\boldsymbol{\omega}}(f\circ\mathbf{x}^*) = \frac{1}{n}\sum_{j=0}^{n-1} f\circ\mathbf{x}^*\Big(\frac{j}{n}\Big)\exp\Big(-2i\pi j\frac{\mathbf{k}\cdot\boldsymbol{\omega}}{n}\Big)$$

is the complex discrete Fourier coefficient of the one-dimensional function $f\circ\mathbf{x}^*$. In the sequel, the dependence on n, $\boldsymbol{\omega}$ and $\boldsymbol{\varphi}$ is generally omitted for convenience.

3.1.2 Estimation

The estimators of $\mathrm{V}_{\mathfrak{u}}(f)$, $\mathrm{V}(f)$ and consequently of $\mathrm{S}_{\mathfrak{u}}(f)$ were introduced by using the approximation in (11) (see [8] and Appendix C in [9]). On the one hand, for any non-empty subset $\mathfrak{u} \subseteq \{1, \ldots, d\}$ and any finite subset $K_{\mathfrak{u}} \subseteq \mathbb{Z}^*_{\mathfrak{u}}$, (11) leads to the definition of the estimator of $\mathrm{V}_{\mathfrak{u}}(f)$

$$\widehat{\mathrm{V}}_{\mathfrak{u}}^{\mathrm{FAST}}(f, K_{\mathfrak{u}}, \mathbf{x}^*) = \sum_{\mathbf{k} \in K_{\mathfrak{u}}} \left|\widehat{\mathrm{c}}_{\mathbf{k}\cdot\boldsymbol{\omega}}(f \circ \mathbf{x}^*)\right|^2. \tag{12}$$

On the other hand, (11) gives

$$\begin{aligned} \mathrm{V}(f) &= \mathrm{c}_{\mathbf{0}}(f^2) - \mathrm{c}_{\mathbf{0}}(f)^2 \\ &\approx \widehat{\mathrm{c}}_0(f^2 \circ \mathbf{x}^*) - \widehat{\mathrm{c}}_0(f \circ \mathbf{x}^*)^2 \end{aligned}$$

and Parseval's identity leads to the definition of the estimator of $\mathrm{V}(f)$

$$\widehat{\mathrm{V}}^{\mathrm{FAST}}(f, \mathbf{x}^*) = \sum_{k=1}^{n-1} \left|\widehat{\mathrm{c}}_k(f \circ \mathbf{x}^*)\right|^2.$$

This naturally leads to the estimator of the variance-based sensitivity indices $\mathrm{S}_{\mathfrak{u}}(f)$

$$\widehat{\mathrm{S}}_{\mathfrak{u}}^{\mathrm{FAST}}(f, K_{\mathfrak{u}}, \mathbf{x}^*) = \frac{\displaystyle\sum_{\mathbf{k} \in K_{\mathfrak{u}}} \left|\widehat{\mathrm{c}}_{\mathbf{k}\cdot\boldsymbol{\omega}}(f \circ \mathbf{x}^*)\right|^2}{\displaystyle\sum_{k=1}^{n-1} \left|\widehat{\mathrm{c}}_k(f \circ \mathbf{x}^*)\right|^2}.$$

As in Example 2, note that by Parseval's identity $\widehat{\mathrm{V}}^{\mathrm{FAST}}(f, \mathbf{x}^*)$ is equal to the empirical variance $\widehat{\mathrm{V}}(f, \{\mathbf{x}^*(\frac{j}{n})\}_{j=0..n-1})$.

3.1.3 Choice of parameters $\boldsymbol{\omega}$ and n

As discussed by Schaibly and Shuler [31] and Cukier et al. [10], $\boldsymbol{\omega}$ and n should be correctly chosen so as to minimize the cubature error in the approximation in (11). In order to avoid interferences i.e.

$$\mathbf{k} \cdot \boldsymbol{\omega} - \mathbf{k}' \cdot \boldsymbol{\omega} = 0 \quad \text{for } \mathbf{k},\, \mathbf{k}' \in \mathbb{Z}^d,\, \mathbf{k} \neq \mathbf{k}'$$

and aliasing i.e.

$$\mathbf{k} \cdot \boldsymbol{\omega} - \mathbf{k}' \cdot \boldsymbol{\omega} = jn \quad \text{for } \mathbf{k},\, \mathbf{k}' \in \mathbb{Z}^d,\, \mathbf{k} \neq \mathbf{k}' \text{ and } j \in \mathbb{Z}^*$$

— that both lead to $\widehat{\mathrm{c}}_{\mathbf{k}\cdot\boldsymbol{\omega}}(f \circ \mathbf{x}^*) = \widehat{\mathrm{c}}_{\mathbf{k}'\cdot\boldsymbol{\omega}}(f \circ \mathbf{x}^*)$ — Schaibly and Shuler [31] propose to choose ω_1, $\ldots$, ω_d free of interferences up to order $N \in \mathbb{N}^*$:

$$(\mathbf{k} - \mathbf{k}') \cdot \boldsymbol{\omega} \neq 0 \quad \text{for all } \mathbf{k},\ \mathbf{k}' \in \mathbb{Z}^d,\ \mathbf{k} \neq \mathbf{k}', \text{ s.t. } \sum_{i=1}^{d} |k_i - k'_i| \leq N + 1 \tag{13}$$

and n sufficiently large

$$n \approx N \max(\omega_1, \dots, \omega_d). \tag{14}$$

More recently, referring to the classical information theory, Saltelli et al. [30] suggest to replace (14) with Nyquist-Shannon sampling theorem (see e.g. [24])

$$n > 2N \max(\omega_1, \dots, \omega_d). \tag{15}$$

In our opinion, the criterion stated in (13) should be written

$$(\mathbf{k} - \mathbf{k}') \cdot \boldsymbol{\omega} \neq 0 \quad \text{for all } \mathbf{k},\ \mathbf{k}' \in \mathbb{Z}^d,\ \mathbf{k} \neq \mathbf{k}', \text{ s.t. } \sum_{i=1}^{d} |k_i| \leq N' \text{ and } \sum_{i=1}^{d} |k'_i| \leq N' \tag{16}$$

since the main objective is to avoid interferences within a finite subset of $\mathbb{Z}^d$ out of which the Fourier coefficients of f are a priori negligible — in (16), this subset is the closed l^1-norm ball of radius N'. Thus we may reformulate the whole criterion stated in (13) and (15) with respect to the set $K = \sqcup_{\mathfrak{u}} K_{\mathfrak{u}}$ where the $K_{\mathfrak{u}}$'s are the truncation sets in the FAST estimator of $\mathrm{V}_{\mathfrak{u}}(f)$ given in (12). We propose to choose $\omega_1, \dots, \omega_d$ free of interferences within K i.e.

$$(\mathbf{k} - \mathbf{k}') \cdot \boldsymbol{\omega} \neq 0 \ \text{ for all } \mathbf{k},\ \mathbf{k}' \in K,\ \mathbf{k} \neq \mathbf{k}' \quad \text{and} \quad n > \max_{\mathbf{k},\mathbf{k}' \in K} \big((\mathbf{k} - \mathbf{k}') \cdot \boldsymbol{\omega}\big). \tag{17}$$

In the sequel, we refer to the latter as the "classic" criterion of FAST.

3.2 Review of RBD

RBD makes use of the previous framework setting $\boldsymbol{\varphi} = \mathbf{0}$, $\omega_1 = \dots = \omega_d = \omega \in \mathbb{N}^*$ — usually set to 1 — and applying random permutations on the coordinates of the resulting points $\mathbf{x}^*(\frac{j}{n})$. More precisely, let $\sigma_1, \dots, \sigma_d$ be random permutations on $\{0, \dots, n-1\}$ and $\mathfrak{S}$ denote the set of all possible $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_d)$. Given $\boldsymbol{\sigma} \in \mathfrak{S}$, consider the function $\mathbf{x}^\times = (x_1^\times, \dots, x_d^\times)$ defined on $\{0, \frac{1}{n}, \dots, \frac{n-1}{n}\}$ such that for all $i \in \{1, \dots, d\}$ and $j \in \{0, \dots, n-1\}$,

$$x_i^\times\Big(\frac{j}{n}\Big) = \frac{1}{\pi} \arcsin\Big(\sin\Big(2\pi\omega \frac{\sigma_i(j)}{n}\Big)\Big) + \frac{1}{2}.$$

Thus denoting σ_i^{-1} the inverse permutation of σ_i, define

$$\mathbf{x}^{\times,i}\Big(\frac{j}{n}\Big) = \mathbf{x}^\times\Big(\frac{\sigma_i^{-1}(j)}{n}\Big).$$

Finally through a heuristic argument Tarantola et al. [38] introduce the RBD estimators of $\mathrm{V}_{\mathfrak{u}}(f)$, $\mathrm{V}(f)$ and $\mathrm{S}_{\mathfrak{u}}(f)$ for first-order terms — i.e. $\mathfrak{u} = \{i\}$, $i \in \{1, \dots, d\}$ —. For any finite subset $K_{\{i\}} \subseteq \mathbb{Z}^*_{\{i\}}$, we have

$$\widehat{\mathrm{V}}_i^{\mathrm{RBD}}(f, K_{\{i\}}, \mathbf{x}^\times) = \sum_{\mathbf{k} \in K_{\{i\}}} \big|\widehat{\mathrm{c}}_{k_i\omega}(f \circ \mathbf{x}^{\times,i})\big|^2,$$

$$\widehat{\mathrm{V}}^{\mathrm{RBD}}(f,\mathbf{x}^{\times}) = \sum_{k=1}^{n-1} \left|\widehat{\mathrm{c}}_k(f\circ\mathbf{x}^{\times})\right|^2.$$

and

$$\widehat{\mathrm{S}}_i^{\mathrm{RBD}}(f,K_{\{i\}},\mathbf{x}^{\times}) = \frac{\displaystyle\sum_{\mathbf{k}\in K_{\{i\}}} \left|\widehat{\mathrm{c}}_{k_i\omega}(f\circ\mathbf{x}^{\times,i})\right|^2}{\displaystyle\sum_{k=1}^{n-1}\left|\widehat{\mathrm{c}}_k(f\circ\mathbf{x}^{\times})\right|^2}.$$

As in FAST note that by Parseval's identity, the estimator $\widehat{\mathrm{V}}^{\mathrm{RBD}}(f,\mathbf{x}^{\times})$ is equal to the empirical variance $\widehat{\mathrm{V}}(f,\{\mathbf{x}^{\times}(\frac{j}{n})\}_{j=0..n-1})$. In the sequel, the dependence on ω and $\boldsymbol{\sigma}$ is generally omitted for convenience.

3.3 FAST and RBD revisited

3.3.1 Main result

First we introduce more notation. For any $p\in\mathbb{N}^*$, let

$$\begin{array}{rccl} r_p: & [0,1] & \longrightarrow & [0,1] \\ & x & \longmapsto & \left\{\begin{array}{ll} 2\{px\} & \text{if } 0\le\{px\}<\frac{1}{2} \\ 2-2\{px\} & \text{if } \frac{1}{2}\le\{px\}\le 1 \end{array}\right. \end{array}$$

and for any $\varphi\in[0,2\pi)$

$$\begin{array}{rccl} t_\varphi: & [0,1] & \longrightarrow & [0,1] \\ & x & \longmapsto & \{x+\tilde\varphi\} \quad \text{with } \tilde\varphi = \frac{1}{4}+\frac{\varphi}{2\pi}\ . \end{array}$$

Then we define the linear operators $\mathcal{R}_p$ and $\mathcal{T}_{\boldsymbol{\varphi}}$ (see Figure 1) on $L^2([0,1]^d)$ such that for all $\mathbf{x}\in[0,1]^d$,

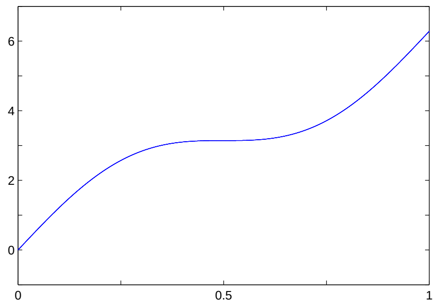
$$\mathcal{R}_p f(\mathbf{x}) = f\big(r_p(x_1)\dots,r_p(x_d)\big) \ \ \text{et} \ \ \mathcal{T}_{\boldsymbol{\varphi}} f(\mathbf{x}) = f\big(t_{\varphi_1}(x_1),\dots,t_{\varphi_d}(x_d)\big).$$

and note that $\mathcal{R}_p = \underbrace{\mathcal{R}_1\circ\cdots\circ\mathcal{R}_1}_{p \text{ times}}$. We also introduce two classical designs of experiments. For any $\boldsymbol{\omega}\in(\mathbb{N}^*)^d$, we denote

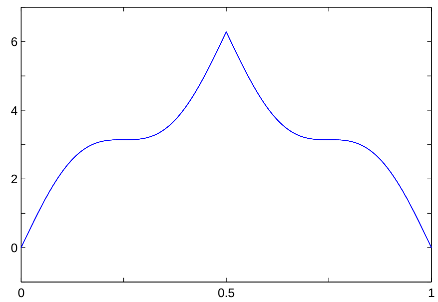
$$G(\boldsymbol{\omega}) = \left\{\Big(\Big\{\frac{j}{n}\omega_1\Big\},\dots,\Big\{\frac{j}{n}\omega_d\Big\}\Big),\ j\in\{0,\dots,n-1\}\right\}.$$

the cyclic subgroup — of order $n/gcd(\omega_1,\dots,\omega_d,n)$ — of the torus $\mathbb{T}^d=(\mathbb{R}/\mathbb{Z})^d\simeq[0,1)^d$ generated by $(\{\frac{\omega_1}{n}\},\dots,\{\frac{\omega_d}{n}\})$ (see e.g. [15]). For any $\boldsymbol{\sigma}\in\mathfrak{S}$ we also denote

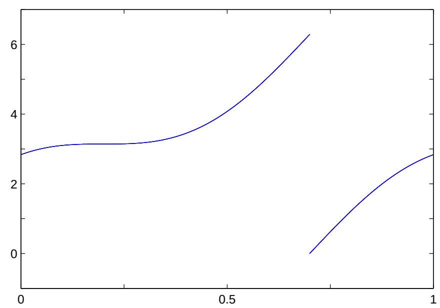
$$A(\boldsymbol{\sigma}) = \left\{\Big(\frac{\sigma_1(j)}{n},\dots,\frac{\sigma_d(j)}{n}\Big),\ j\in\{0,\dots,n-1\}\right\}$$



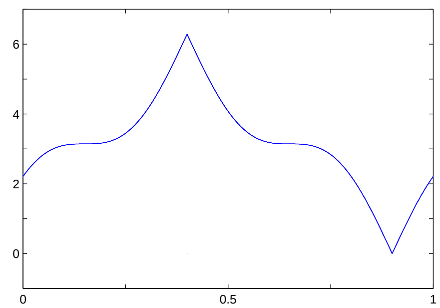
(a) Plot of $f : x \mapsto x + \sin(x)$



(b) Plot of $\mathcal{R}_1 f$



(c) Plot of $\mathcal{T}_{\frac{\pi}{10}} f$



(d) Plot of $(\mathcal{T}_{\frac{\pi}{30}} \circ \mathcal{R}_1) f$

Figure 1: Examples of operators $\mathcal{R}_p$ and $\mathcal{T}_{\boldsymbol{\varphi}}$ in dimension 1.

the orthogonal array of strength 1 and index unity with elements taken from $\{0, \frac{1}{n}, \dots, \frac{n-1}{n}\}$ and based on the permutation σ (see e.g. [16]). FAST and RBD methods are now introduced in a new way by using the basic estimator in (8).

Proposition 2. *Let $f : [0,1]^d \to \mathbb{R}$ be a square-integrable function. For any non-empty subset $\mathfrak{u} \subseteq \{1, \dots, d\}$, any finite subset $K_{\mathfrak{u}} \subseteq \mathbb{Z}^*_{\mathfrak{u}}$, $\boldsymbol{\varphi} \in [0, 2\pi)^d$ and $\boldsymbol{\omega} \in (\mathbb{N}^*)^d$, we have*

$$\widehat{\mathrm{S}}_{\mathfrak{u}}^{\mathrm{FAST}}(f, K_{\mathfrak{u}}, \mathbf{x}^*) = \widehat{\mathrm{S}}_{\mathfrak{u}}\big((\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1) f, K_{\mathfrak{u}}, G(\boldsymbol{\omega})\big). \tag{18}$$

For any $i \in \{1, \dots, d\}$, any finite subset $K_{\{i\}} \subseteq \mathbb{Z}^*_{\{i\}}$, $\boldsymbol{\sigma} \in \mathfrak{S}$ and $\omega \in \mathbb{N}^*$, we have

$$\widehat{\mathrm{S}}_{i}^{\mathrm{RBD}}(f, K_{\{i\}}, \mathbf{x}^{\times}) = \widehat{\mathrm{S}}_{i}\big((\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_{\omega}) f, \omega K_{\{i\}}, A(\boldsymbol{\sigma})\big). \tag{19}$$

where $\tilde{\boldsymbol{\omega}} = \left(\frac{(1-\omega)\pi}{2\omega}, \cdots, \frac{(1-\omega)\pi}{2\omega}\right)$ and $\omega K_{\{i\}} = \{(\omega k_1, \dots, \omega k_d),\ \mathbf{k} \in K_{\{i\}}\}$.

Proof. It essentially consists in showing that for all $j \in \{0, \dots n-1\}$

$$f \circ \mathbf{x}^*\Big(\frac{j}{n}\Big) = (\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1) f\Big(\Big\{\frac{j}{n}\omega_1\Big\}, \dots, \Big\{\frac{j}{n}\omega_d\Big\}\Big)$$

and

$$f \circ \mathbf{x}^{\times}\Big(\frac{j}{n}\Big) = (\mathcal{T}_{\tilde{\omega}} \circ \mathcal{R}_{\omega}) f\Big(\frac{\sigma_1(j)}{n}, \dots, \frac{\sigma_d(j)}{n}\Big).$$

See details in Appendix A.1. $\square$

Remark 1. *In the RBD method, the parameter ω is usually set to 1 but its role is not well understood up to now. In our opinion there is no reason to set $\omega \neq 1$ since if $gcd(\omega, n) = 1$ then it leads to the case $\omega = 1$, and otherwise the estimator in (19) is potentially less efficient than in the case $\omega = 1$ (see details in Appendix A.2.).*

3.3.2 What FAST and RBD are

It is clear from Proposition 2 that FAST and RBD only consists in applying the basic estimator introduced in (8) to a particular transform $(\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_p)f$ of the function f and a particular design of experiments $G(\boldsymbol{\omega})$ or $A(\boldsymbol{\sigma})$. Now it is also clear that the basic estimator generates an error term due to truncations — in (6) — and an other one due to numerical integrations — in (5) and (7). Moreover, the use of $(\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_p)f$ instead of f could also have an impact on the sensitivity indices estimation error. We now investigate this latter issue by introducing the notion of invariance of the variance decomposition.

Definition 1. *Let $\mathcal{L}$ be a linear operator on $L^2([0,1]^d)$. The variance decomposition is said to be $\mathcal{L}$-invariant on $L^2([0,1]^d)$ if for any non-empty set $\mathfrak{u} \subseteq \{1, \dots, d\}$ and any function $f \in L^2([0,1]^d)$ we have*

$$\mathrm{V}_{\mathfrak{u}}(\mathcal{L}f) = \mathrm{V}_{\mathfrak{u}}(f).$$

This leads to the following result

Lemma 1. *For any $p \in \mathbb{N}^*$ and any $\boldsymbol{\varphi} \in [0, 2\pi)^d$, the variance decomposition is $\mathcal{R}_p$ and $\mathcal{T}_{\boldsymbol{\varphi}}$-invariant on $L^2([0,1]^d)$.*

Proof. See Appendix A.3. $\square$

As a consequence, for any non-empty subset $\mathfrak{u} \subseteq \{1, \dots, d\}$, we have

$$\mathrm{S}_{\mathfrak{u}}\big((\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_p)f\big) = \mathrm{S}_{\mathfrak{u}}(f)$$

and this asserts the validity of FAST and RBD methods. Note that the linear operator $\mathcal{R}_p$ "regularize" the function f in the sense that if $\mathbf{x} \mapsto f(\mathbf{x})$ is continuous on $[0,1]^d$ and $\mathbf{x} \to f(\{x_1\}, \dots, \{x_d\})$

is discontinuous on $\mathbb{R}^d$ then $\mathbf{x} \to \mathcal{R}_p f(\{x_1\}, \ldots, \{x_d\})$ is continuous on $\mathbb{R}^d$. This is an important property since by Riemann-Lebesgue lemma $|\mathrm{c}_{\mathbf{k}}(f)|$ converges to 0 as $||\mathbf{k}||$ tends to ∞, and the smoother the function f, the faster the convergence (see e.g. [45]). The other operator $\mathcal{T}_{\boldsymbol{\varphi}}$ essentially allows to define randomized estimators in FAST.

3.3.3 Potential generalizations

To end with, we list three natural generalizations that are further discussed in the next section:

- the estimator $\widehat{\mathrm{S}}_{\mathrm{u}}\big((\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1)f, K_{\mathrm{u}}, G(\boldsymbol{\omega})\big)$ can also be defined for a group G of any rank $r \leq d$
- the estimator $\widehat{\mathrm{S}}_i\big((\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_\omega)f, \omega K_{\{i\}}, A(\boldsymbol{\sigma})\big)$ can also be defined for a sensitivity index of any order: $\widehat{\mathrm{S}}_{\mathrm{u}}\big((\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_\omega)f, \omega K_{\mathrm{u}}, A(\boldsymbol{\sigma})\big)$, note that it has been already applied in [44]
- the latter estimator $\widehat{\mathrm{S}}_{\mathrm{u}}\big((\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_\omega)f, \omega K_{\mathrm{u}}, A(\boldsymbol{\sigma})\big)$ can also be defined for an orthogonal array A having any parameters.

4 Error analysis

For convenience, operators $\mathcal{T}_{\boldsymbol{\varphi}}$ and $\mathcal{R}_p$ are now omitted. Moreover, we assume that the function f has an absolutely convergent Fourier representation, i.e. $\sum\limits_{\mathbf{k} \in \mathbb{Z}^d} |\mathrm{c}_{\mathbf{k}}(f)| < +\infty$.

4.1 Cubature error in FAST

4.1.1 Two points of view

In this section we mainly focus on the error term

$$e_{\mathbf{k}}(f, G) = \widehat{\mathrm{c}}_{\mathbf{k}}(f, G) - \mathrm{c}_{\mathbf{k}}(f) \tag{20}$$

where G is a subgroup of $\mathbb{T}^d$ of order n and $\mathbf{k} \in \mathbb{Z}^d$. By its definition, the term $\widehat{\mathrm{c}}_{\mathbf{k}}(f, G)$ consists of an equal weight cubature rule at the n nodes of the group G, also known as a lattice rule (see [33] for a survey). Moreover by the generalized Poisson summation formula (see e.g. [23]), the error term in (20) is precisely

$$e_{\mathbf{k}}(f, G) = \sum_{\mathbf{h} \in G^\perp \setminus \{\mathbf{0}\}} \mathrm{c}_{\mathbf{k}+\mathbf{h}}(f) \tag{21}$$

where $G^\perp = \{\mathbf{h} \in \mathbb{Z}^d \mid \forall \mathbf{x} \in G,\ \mathbf{h} \cdot \mathbf{x} \equiv 0 \pmod 1\}$ is the subgroup of $\mathbb{Z}^d$ orthogonal to G, also known as the dual lattice of G.

In the lattice rules field, $e_{\mathbf{0}}(f, G)$ is the only term of interest, and there exist two main points of view to control it. One consists in looking for "good" groups G such that the cubature rule is exact for a set of trigonometric polynomials, i.e. for a finite subset K of $\mathbb{Z}^d$,

$$e_{\mathbf{0}}(f, G) = 0 \text{ for all } f \text{ such that } \forall \mathbf{k} \notin K,\ \mathrm{c}_{\mathbf{k}}(f) = 0\ .$$

The other point of view aims to find "good" groups G such that the cubature rule has an absolute error $|e_{\mathbf{0}}(f, G)|$ dominated by an explicit bound for all f in a particular space of smooth functions. Note that these approaches are compatible to each other (see e.g. [7] and the references therein).

Now concerning the study of error in FAST, the first point of view, which essentially corresponds to the classic FAST, consists of a trigonometric interpolation issue and leads to a metamodel approach of the estimation of the sensitivity indices. The second one, which is more original, allows to derive error bounds for $\widehat{\mathrm{V}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, G)$ and $\widehat{\mathrm{V}}(f, G)$ in spaces of smooth functions. Both these methods are discussed below.

4.1.2 Metamodel approach

Let K be a finite subset of $\mathbb{Z}^d$. Then an immediate consequence of (21) is that a group G satisfies the property

$$e_{\mathbf{k}}(f, G) = 0 \text{ for all } \mathbf{k} \in K \text{ and for all } f \text{ such that } \forall \mathbf{k} \notin K,\ \mathrm{c}_{\mathbf{k}}(f) = 0$$

if and only if

$$\forall \mathbf{k}, \mathbf{k}' \in K, \mathbf{k} \neq \mathbf{k}',\ \exists \mathbf{x} \in G,\ (\mathbf{k} - \mathbf{k}') \cdot \mathbf{x} \not\equiv 0 \pmod 1\ . \tag{22}$$

More fundamentally, for any $E \subseteq \mathbb{Z}^d$, consider the trigonometric polynomial

$$\tilde{f}_E(\mathbf{x}) = \sum_{\mathbf{k} \in E} \widehat{\mathrm{c}}_{\mathbf{k}}(f, G) \exp(2i\pi \mathbf{k} \cdot \mathbf{x})\ , \tag{23}$$

then the equivalence above leads to the following result

Proposition 3. *Let G be a subgroup of the torus $\mathbb{T}^d$ of order $|G| = n$ and $K = \cup_{\mathfrak{u} \neq \emptyset} K_{\mathfrak{u}}$ satisfying the criterion* (22) *where for all non-empty subsets $\mathfrak{u}$ of $\{1, \ldots, d\}$, $K_{\mathfrak{u}} \subseteq \mathbb{Z}^*_{\mathfrak{u}}$*

i) *if $|K| = n$, then $\tilde{f}_K$ is a trigonometric interpolation polynomial of f at the n nodes $\mathbf{x} \in G$ and we have*

$$\widehat{\mathrm{S}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, G) = \mathrm{S}_{\mathfrak{u}}(\tilde{f}_K).$$

ii) *if* $|K| < n$, *let* H *be any subset of* $\mathbb{Z}^d$ *such that* $K \subseteq H$, H *satisfies the criterion* (22) *and* $|H| = n$. *Then* $\tilde{f}_H$ *is a trigonometric interpolation polynomial of* f *at the* n *nodes* $\mathbf{x} \in G$ *and we have*

$$\widehat{\mathrm{V}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, G) = \mathrm{V}_{\mathfrak{u}}(\tilde{f}_K) \text{ and } \widehat{\mathrm{V}}(f, G) = \mathrm{V}(\tilde{f}_H).$$

Proof. The only difficulty is to prove that the trigonometric polynomials $\tilde{f}_K$ in the assertion i) and $\tilde{f}_H$ in the assertion ii) are interpolation polynomials at the points $\mathbf{x} \in G$. We demonstrate it for $\tilde{f}_K$, the proof for $\tilde{f}_H$ is exactly the same.

Since the function f has absolutely convergent Fourier representation, we can write

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^d} \mathrm{c}_{\mathbf{k}}(f) \exp(2i\pi \mathbf{k} \cdot \mathbf{x}) = \sum_{\mathbf{k} \in K} \sum_{\mathbf{h} \in G^\perp} \mathrm{c}_{\mathbf{k}+\mathbf{h}}(f) \exp\big(2i\pi(\mathbf{k}+\mathbf{h}) \cdot \mathbf{x}\big) \tag{24}$$

(see details in Appendix A.4) and by definition of $G^\perp$, we have that for any $\mathbf{x} \in G$,

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in K} \sum_{\mathbf{h} \in G^\perp} \mathrm{c}_{\mathbf{k}+\mathbf{h}}(f) \exp(2i\pi \mathbf{k} \cdot \mathbf{x}).$$

The conclusion follows from the definition in (23) since (20) and (21) give

$$\sum_{\mathbf{h} \in G^\perp} \mathrm{c}_{\mathbf{k}+\mathbf{h}}(f) = \widehat{\mathrm{c}}_{\mathbf{k}}(f, G).$$

$\square$

From this point of view, FAST returns analytical values from trigonometric metamodels of the function $(\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1) f$ and the error analysis should be performed on the metamodel itself.

In practice, a set of a priori non-negligible frequencies $K = \cup_{\mathfrak{u} \neq \emptyset} K_{\mathfrak{u}}$ is given and a group G satisfying the criterion (22) and with the smallest order $|G| = n$ has to be found. Searching for this group G is computationaly expensive and may rapidly become unfeasible. One of the cheapest way is to look for cyclic groups $G = G(\boldsymbol{\omega})$, coming back to the classic FAST. In this case, the criterion (22) simply reads

$$\forall \mathbf{k}, \mathbf{k}' \in K, \mathbf{k} \neq \mathbf{k}',\ (\mathbf{k} - \mathbf{k}') \cdot \boldsymbol{\omega} \not\equiv 0 \pmod{n}\ . \tag{25}$$

Note that this new criterion plays the same role as the classic criterion of FAST given in (17). The main difference between these two approaches is that optimization on n is performed in (25), consequently this new criterion allows to find group G with smaller order n. We illustrate the efficiency of both criterions by using basic exhaustive algorithms with computational complexity $O(n^d)$. The results are gathered in Table 1 and show that the new criterion leads to a non-negligible improvement.

		$d=2$			$d=3$			$d=4$			$d=5$		
$N1$	N_2	$\|K\|$	n_{old}	n_{new}	$\|K\|$	n_{old}	n_{new}	$\|K\|$	n_{old}	n_{new}	$\|K\|$	n_{old}	n_{new}
4	2	20	41	29	36	65	50	56	105	63	80	177	111
5	3	32	61	48	66	141	102	112	241	173	170	471	302
6	4	48	85	65	108	241	155	192	541	323	300	997	613
7	5	68	113	89	162	421	284	296	1177	586	470	1891	1279
8	6	92	145	120	228	625	429	424	1985	1033	680	3457	2222
9	7	120	181	149	306	937	645	576	3007	1706	930	–	–
10	8	152	221	185	396	1281	933	752	4501	2529	1220	–	–
11	9	188	265	228	498	1805	1284	952	7261	3684	1550	–	–

Table 1: Comparison in dimension $d = 2$, 3, 4 and 5 between the minimum sample size n given by the classic criterion of FAST (denoted n_{old}) and the new one proposed in (25) (denoted n_{new}). Here, the $K_{\{i\}}$'s are equal to $\mathbb{Z}^*_{\{i\}} \cap \{|k_i| \leq N_1\}$, the $K_{\{i,j\}}$'s are equal to $\mathbb{Z}^*_{\{i,j\}} \cap \{|k_i| + |k_j| \leq N_2\}$ and for all $\mathfrak{u}$ such that $|\mathfrak{u}| > 2$, $K_\mathfrak{u} = \emptyset$. Such sets K are particularly well-suited to analyse functions whose effective dimension is less than 2 — see Definition 4 in Section 4.2.2.

Remark 2. *Even if cyclic groups seem to be suitable in the previous issue, the computational cost of the research of a generator $\boldsymbol{\omega}$ can become prohibitive in high-dimensional problems. In this case, alternative algorithms can be used instead of a systematic research technique (for a recent reference, see e.g.* [20]*).*

4.1.3 Error bounds

Searching for a finite subgroup G of the torus $\mathbb{T}^d$ such that $e_\mathbf{0}(f, G)$ has an explicit bound in a particular function space is a problem known as the construction of good lattice rules (for a survey see [33] or more recently [25]). Most of the results in this field are established in Korobov spaces which are suitable to handle lattice methods; so we derive error bounds for sensitivity indices in these spaces. For $\alpha > 1$ and $\boldsymbol{\gamma} = (\gamma_\mathfrak{u})_{\mathfrak{u} \subseteq \{1,\dots,d\}}$ with non-negative $\gamma_\mathfrak{u}$'s, define the weighted Korobov space $\mathcal{H}_{\alpha,\boldsymbol{\gamma}}$ to be the Hilbert space with reproducing kernel

$$RK_{\alpha,\boldsymbol{\gamma}}(\mathbf{x}, \mathbf{y}) = 1 + \sum_{\mathbf{k} \in (\mathbb{Z}^d)^*} r(\mathbf{k}, \alpha, \boldsymbol{\gamma})^{-1} \exp\big(2i\pi \mathbf{k} \cdot (\mathbf{x} - \mathbf{y})\big)$$

where for any $\mathbf{k} \neq \mathbf{0}$, $r(\mathbf{k}, \alpha, \boldsymbol{\gamma}) = \gamma_{\mathfrak{u}_\mathbf{k}}^{-1} \prod_{i \in \mathfrak{u}_\mathbf{k}} |k_i|^\alpha$, where $\mathfrak{u}_\mathbf{k}$ is such that $\mathbf{k} \in \mathbb{Z}^*_{\mathfrak{u}_\mathbf{k}}$. For $\mathbf{k}$ such that $\gamma_{\mathfrak{u}_\mathbf{k}} = 0$, we set by convention $r(\mathbf{k}, \alpha, \boldsymbol{\gamma}) = \infty$. Thus the kernel can be rewritten

$$RK_{\alpha,\boldsymbol{\gamma}}(\mathbf{x}, \mathbf{y}) = 1 + \sum_{\substack{\mathbf{k} \in (\mathbb{Z}^d)^* \\ \gamma_{\mathfrak{u}_\mathbf{k}} \neq 0}} r(\mathbf{k}, \alpha, \boldsymbol{\gamma})^{-1} \exp\big(2i\pi \mathbf{k} \cdot (\mathbf{x} - \mathbf{y})\big)$$

and we deduce that the norm of $f \in \mathcal{H}_{\alpha,\boldsymbol{\gamma}}$ satisfies

$$||f||^2_{\mathcal{H}_{\alpha,\boldsymbol{\gamma}}} = \mathrm{c}_{\mathbf{0}}(f)^2 + \sum_{\substack{\mathbf{k}\in(\mathbb{Z}^d)^* \\ \gamma_{\mathfrak{u}_{\mathbf{k}}}\neq 0}} r(\mathbf{k},\alpha,\boldsymbol{\gamma})|\mathrm{c}_{\mathbf{k}}(f)|^2 < +\infty$$

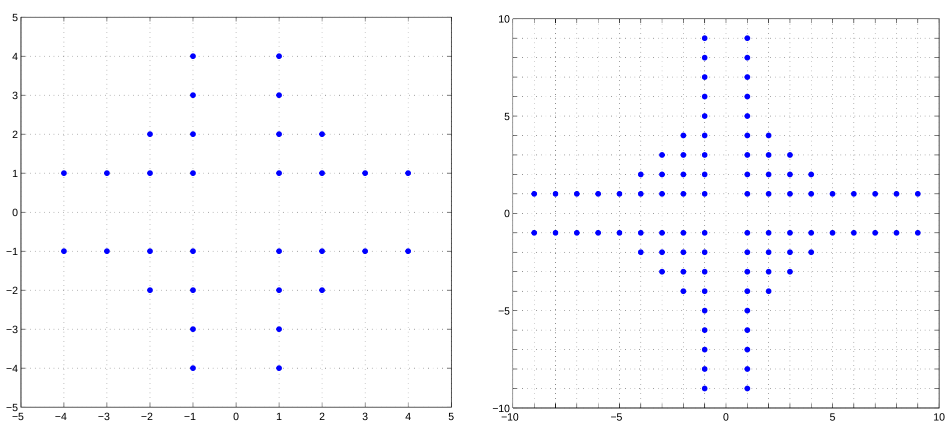
and consequently

$$\forall \mathbf{k} \in (\mathbb{Z}^d)^* \text{ such that } \gamma_{\mathfrak{u}_{\mathbf{k}}} \neq 0,\ |\mathrm{c}_{\mathbf{k}}(f)|^2 \leq \frac{\gamma_{\mathfrak{u}_{\mathbf{k}}}||f||^2_{\mathcal{H}_{\alpha,\boldsymbol{\gamma}}}}{\prod_{i\in\mathfrak{u}_{\mathbf{k}}}|k_i|^\alpha}.$$

Note that for any $\mathbf{k} \in (\mathbb{Z}^d)^*$ such that $\gamma_{\mathfrak{u}_{\mathbf{k}}} = 0$, $f \in \mathcal{H}_{\alpha,\boldsymbol{\gamma}}$ implies $\mathrm{c}_{\mathbf{k}}(f) = 0$. We also make a restriction on the sets of frequencies $K_{\mathfrak{u}}$'s. Here we assume that for any non-empty set $\mathfrak{u} \subseteq \{1,\dots,d\}$, $K_{\mathfrak{u}}$ is of Zaremba cross-type (see Figure 2)

$$K_{\mathfrak{u}} = \mathcal{Z}_{\mathfrak{u},\beta_{\mathfrak{u}}} = \left\{ \mathbf{k} \in \mathbb{Z}^*_{\mathfrak{u}},\ \prod_{i\in\mathfrak{u}}|k_i| \leq \beta_{\mathfrak{u}} \right\}$$

where $\beta_{\mathfrak{u}} \geq 1$. This kind of sparse grids is particularly well-suited for the analysis of high-dimensional smooth functions. We now give the result on error bounds for $\widehat{\mathrm{V}}_{\mathfrak{u}}(f,K_{\mathfrak{u}},G)$ and $\widehat{\mathrm{V}}(f,G)$ in $\mathcal{H}_\alpha$.



(a) Plot of $\mathcal{Z}_{\{1,2\},4}$ (b) Plot of $\mathcal{Z}_{\{1,3\},9}$

Figure 2: Illustration of crosses $\mathcal{Z}_{\mathfrak{u},\beta_{\mathfrak{u}}}$.

Proposition 4. *Let $f \in \mathcal{H}_{\alpha,\boldsymbol{\gamma}}$ with $\alpha > 2$ and $\boldsymbol{\gamma} = (\gamma_{\mathfrak{u}})_{\mathfrak{u}\subseteq\{1,\dots,d\}}$ with non-negative components. Let G be a subgroup of $\mathbb{T}^d$ of order n such that the cubature error related to G is dominated by the explicit bound $B(\alpha,n,d,\boldsymbol{\gamma})$ on the unit ball of $\mathcal{H}_{\alpha,\boldsymbol{\gamma}}$ i.e. for all f in $\mathcal{H}_{\alpha,\boldsymbol{\gamma}}$, $|\widehat{\mathrm{c}}_{\mathbf{0}}(f,G) - \mathrm{c}_{\mathbf{0}}(f)| \leq B(\alpha,n,d,\boldsymbol{\gamma})||f||_{\mathcal{H}_{\alpha,\boldsymbol{\gamma}}}$. Then*

i) if there exists $\alpha' > 2$ and $\boldsymbol{\gamma}' = (\gamma'_{\mathfrak{u}})_{\mathfrak{u}\subseteq\{1,\dots,d\}}$ with non-negative components such that $f^2 \in \mathcal{H}_{\alpha',\boldsymbol{\gamma}'}$, *we have*

$$\left|\widehat{\mathrm{V}}(f,G)-\mathrm{V}(f)\right| \leq ||f||^2_{\mathcal{H}_\alpha} B(\alpha,n,d,\boldsymbol{\gamma})\big(2+B(\alpha,n,d,\boldsymbol{\gamma})\big) + ||f^2||_{\mathcal{H}_{\alpha'}} B(\alpha',n,d,\boldsymbol{\gamma}')$$

ii) for any non-empty set $\mathfrak{u} \subseteq \{1,\ldots,d\}$ *and* $K_\mathfrak{u} = \mathcal{Z}_{\mathfrak{u},\beta_\mathfrak{u}}$*, we have*

$$\begin{aligned}\left|\widehat{\mathrm{V}}_\mathfrak{u}(f,K_\mathfrak{u},G)-\mathrm{V}_\mathfrak{u}(f)\right| \leq ||f||^2_{\mathcal{H}_{\alpha,\gamma}} \Big[& C(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},|\mathfrak{u}|) + B(\alpha,n,d,\boldsymbol{\gamma})^2 S_1(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u}) \\ &+ B(\alpha,n,d,\boldsymbol{\gamma}) S_2(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u})\Big]\end{aligned}$$

where

$$\begin{aligned}S_1(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u}) &= \gamma_{frac}\sum_{\mathbf{k}\in K_\mathfrak{u}}\prod_{i\in\mathfrak{u}}\big(|k_i|+1\big)^\alpha \quad, \ \gamma_{frac} = \max_{\substack{\mathfrak{u},\mathfrak{v}\subset\{1,\ldots,d\}\\ \gamma_\mathfrak{v}\neq 0}} \gamma_\mathfrak{u}/\gamma_\mathfrak{v} \\ S_2(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u}) &= \gamma_{frac}\gamma_\mathfrak{u}^{1/2} 2^{\alpha|\mathfrak{u}|/2}|K_\mathfrak{u}|\end{aligned}$$

and for $|\mathfrak{u}| \leq 2$*, the truncation error term* $C(\alpha,\beta_\mathfrak{u},|\mathfrak{u}|)$ *are*

$$C(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},1) = \frac{2\gamma_{max}\zeta(\alpha)}{\beta_\mathfrak{u}^{\alpha-1}} \quad, \ \gamma_{max} = \max_{\mathfrak{u}\subset\{1,\ldots,d\}} \gamma_\mathfrak{u} \tag{26}$$

$$C(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},2) = \frac{4\gamma_{max}\big[\zeta(\alpha)^2+\zeta(\alpha)\big(\log(\beta_\mathfrak{u})+2\big)\big]}{\beta_\mathfrak{u}^{\alpha-1}} \ . \tag{27}$$

Proof. See Appendix A.5. □

It is also possible to derive explicit formulas of the truncation error term for $|\mathfrak{u}| > 2$, but this is more complicated and of second interest. Secondly, it has to be noted that, in the second item of Proposition 4, the functions S_1 and S_2 are increasing with respect to the parameter $\beta_\mathfrak{u}$ while the function C is decreasing. As a consequence, efficient bounds consist of a trade-off between $\beta_\mathfrak{u}$ and n such that $B(\alpha,n,d,\boldsymbol{\gamma})^2 S_1(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u})$, $B(\alpha,n,d,\boldsymbol{\gamma})S_2(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u})$ and $C(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},|\mathfrak{u}|)$ have the same order. For example,

i) if $|\mathfrak{u}| = 1$ and $\alpha > 2$, note that $|K_\mathfrak{u}| = 2\beta_\mathfrak{u}$ and deduce $S_1(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u}) \leq 2^{\alpha|\mathfrak{u}|+1}\beta_\mathfrak{u}^{1+\alpha}$, and recall that $C(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},1) = O(\beta_\mathfrak{u}^{1-\alpha})$. Thus the trade-off gives

$$\left|\widehat{\mathrm{V}}_\mathfrak{u}(f,K_\mathfrak{u},G)-\mathrm{V}_\mathfrak{u}(f)\right| = O\Big(B(\alpha,n,d,\boldsymbol{\gamma})^{1-\frac{1}{\alpha}}\Big).$$

ii) if $|\mathfrak{u}| = 2$ and $\alpha > 2$, note that $|K_\mathfrak{u}| \leq 4\beta_\mathfrak{u}(\log(\beta_\mathfrak{u})+1)$ — see argument for (A.21) in Appendix A.5 — and deduce $S_1(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},\mathfrak{u}) \leq 2^{\alpha|\mathfrak{u}|+2}\beta_\mathfrak{u}^{1+\alpha}(\log(\beta_\mathfrak{u})+1)$ and recall that $C(\alpha,\boldsymbol{\gamma},\beta_\mathfrak{u},1) = O\big(\beta_\mathfrak{u}^{1-\alpha}\log(\beta_\mathfrak{u})\big)$. Thus the trade-off gives

$$\left|\widehat{\mathrm{V}}_\mathfrak{u}(f,K_\mathfrak{u},G)-\mathrm{V}_\mathfrak{u}(f)\right| = O\Big(\log\big(B(\alpha,n,d,\boldsymbol{\gamma})^{-1/\alpha}\big)B(\alpha,n,d,\boldsymbol{\gamma})^{1-\frac{1}{\alpha}}\Big).$$

Remark 3. *In unweighted Korobov spaces i.e.* $\boldsymbol{\gamma} = \mathbf{1}$*, it is known that the optimal rate of convergence of a rank-1 lattice rule is*

$$B(\alpha, n, d, \boldsymbol{\gamma}) = O\left(\frac{(\log n)^{d\alpha/2}}{n^{\alpha/2}}\right)$$

(*see e.g.* [33]). *For unweighted Korobov spaces, there exist better rates of convergence for product weights i.e.* $\gamma_{\mathfrak{u}} = \prod_{i\in\mathfrak{u}} \gamma_i$ (*see* [21]) *or for finite-order weights i.e* $\forall\mathfrak{u}$ *with* $|\mathfrak{u}| > d^*$ $(d^* \leq d)$, $\gamma_{\mathfrak{u}} = 0$ (*see* [13]). *The latter are essentially related to an assumption on the effective dimension of* f *in the truncation sense and in the superposition sense, respectively* (*see* [5] *for the definition of effective dimension*).

4.2 Bias in RBD

We now give some results on the well-known issue related to the bias of the estimates in RBD.

4.2.1 Preliminaries

We begin with the definitions of an orthogonal array and the "coincidence defect"

Definition 2. *An orthogonal array in dimension* d*, with* q *levels, strength* $t \leq d$ *and index* λ *is a matrix with* $n = \lambda q^t$ *rows and* d *columns such that in every* n*-by-*t *submatrix each of the* q^t *possible rows — i.e. the distinct* t*-uples* $(l_1, \ldots, l_t)$ *where the* l_i*'s take their values in the set of the* q *levels — occurs exactly the same number* λ *of times.*

Definition 3. *Let* A *be an orthogonal array in dimension* d*, with* q *levels, strength* t *and index* λ*. We say that* A *has the coincidence defect when there exist two rows of* A *that do agree in* $t+1$ *columns; otherwise we say that* A *is defect-free.*

Let $\Pi(q)$ be the set of permutations on $\{0, \frac{1}{q}, \ldots, \frac{q-1}{q}\}$, $\Pi = \Pi(q, d)$ the cartesian product $(\Pi(q))^d$ and $\mu = \mu(q, d)$ the normalized counting measure on $\Pi(q, d)$. Let A be an orthogonal array in dimension d, with q levels $\{0, \frac{1}{q} \ldots, \frac{q-1}{q}\}$, strength t and index λ, and denote $n = \lambda q^t$ its number of rows. For any permutation $\boldsymbol{\pi} = (\pi_1, \ldots \pi_d) \in \Pi$, denote $A(\boldsymbol{\pi})$ the orthogonal array obtained from A after applying each permutation π_j on the levels of the corresponding j-th factor i.e.

$$\text{for all } \ 1 \leq i \leq n \ \text{ and } \ 1 \leq j \leq d, \quad \big(A(\boldsymbol{\pi})\big)_{ij} = \pi_j(A_{ij}) \ .$$

Note that the $A(\boldsymbol{\pi})$'s and A are orthogonal arrays with the same parameters (see [16]). Conversely, it is also easy to show that if A has strength and index equal to 1 — i.e. as in the classic RBD with an odd integer[1] n —; any other orthogonal array A' with the same paramaters as A is of the form $A(\boldsymbol{\pi})$ for a permutation $\boldsymbol{\pi} \in \Pi$. We are now interested in the quantities

$$\mathbb{E}_\mu\left[\widehat{\mathrm{V}}(f, A(\boldsymbol{\pi}))\right] \quad \text{and} \quad \mathbb{E}_\mu\left[\widehat{\mathrm{V}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, A(\boldsymbol{\pi}))\right] ,$$

where $K_{\mathfrak{u}}$ is a finite subset of $\mathbb{Z}_{\mathfrak{u}}^*$.

4.2.2 Bias of the estimator in RBD

Let $\widehat{c}_{\mathbf{k}}(f) = \widehat{c}_{\mathbf{k}}(f, D(q))$ denote the $\mathbf{k}$-th complex discrete Fourier coefficient; we begin with the following important lemma

Theorem 2. [Owen] *Following the previous notation, we have*

$$\mathrm{Var}_\mu\left[\widehat{c}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\right] = \frac{1}{n^2}\sum_{|\mathfrak{u}|>t}\left(\sum_{r=0}^{|\mathfrak{u}|} B(\mathfrak{u}, r)(1-q)^{r-|\mathfrak{u}|}\right)\left(\sum_{\mathbf{k}\in\mathbb{Z}_{\mathfrak{u}}^*(q)} |\widehat{c}_{\mathbf{k}}(f)|^2\right)$$

where

$$B(\mathfrak{u}, r) = \sum_{i=1}^{n}\sum_{j=1}^{n} \mathbf{1}_{|\{l\in\mathfrak{u},\ A_{il}=A_{jl}\}|=r}$$

consists of the number of pairs of rows (A_i, A_j) that match on exactly r of the axes in $\mathfrak{u}$.

Proof. This is exactly Theorem 1 given by Owen in [26]. Just note that, the embedded ANOVA terms on a q^d regular grid — denoted $\beta_{\mathfrak{u}}$ by Owen — are

$$\beta_{\mathfrak{u}}(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}_{\mathfrak{u}}^*(q)} \widehat{c}_{\mathbf{k}}(f)\exp(2i\pi\mathbf{k}\cdot\mathbf{x}).$$

Indeed, for all $\mathbf{x}$ in the regular grid $\{0, \frac{1}{q}, \ldots, \frac{q-1}{q}\}^d$,

$$f(\mathbf{x}) = \sum_{\mathfrak{u}\subseteq\{1,\ldots,d\}} \beta_{\mathfrak{u}}(\mathbf{x})$$

by a trigonometric interpolation argument, and it is also easy to show that the random variables $\beta_{\mathfrak{u}}(X_i,\ i\in\mathfrak{u})$ satisfy the property (2) for independent random variables X_i uniformly distributed on $\{0, \frac{1}{q}\ldots, \frac{q-1}{q}\}$. $\square$

Then we have the following proposition in which the bias of the variance estimate is investigated in unweighted Korobov spaces $\mathcal{H}_\alpha = \mathcal{H}_{\alpha,\mathbf{1}}$ (see Section 4.1.3.)

[1] If n is even, the design of experiments in RBD consists of an orthogonal array with $n/2$ levels, strength 1 and index 2, and may be faced with the coincidence defect.

Proposition 5. *Let A be a defect-free orthogonal array in dimension d with parameters q, t and λ in $\mathbb{N}^*$ with $t < d$. If there exists $\alpha > 2t+1$ such that f and f^2 are in $\mathcal{H}_\alpha$, we have*

$$\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}(f, A(\boldsymbol{\pi}))\Big] = \mathrm{V}(f) - \frac{1}{n}\sum_{1\le|\mathfrak{u}|>t}\mathrm{V}_{\mathfrak{u}}(f) + O\big(n^{-(1+\frac{1}{t})}\big) \ .$$

Proof. See Appendix A.6. □

As a consequence, considering the classic definition of effective dimension in the superposition sense (see e.g. [5])

Definition 4. *The effective dimension of f, in the superposition sense, is the smallest $d_S(f)$ such that*

$$\sum_{1\le|\mathfrak{u}|\le d_S(f)}\mathrm{V}_{\mathfrak{u}}(f) \ge l_S(f)\mathrm{V}(f)$$

where $l_S(f)$ is an arbitrary constant generally set at 0.99.

we have the corollary

Corollary 1. *Under the assumptions of Proposition 5, let $d_S(f)$ and $l_S(f)$ be defined as in Definition 4. If $t \ge d_S$, we have*

$$\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}(f, A(\boldsymbol{\pi}))\Big] = \Big(1 - \frac{\varepsilon}{n}\Big)\mathrm{V}(f) + O\big(n^{-(1+\frac{1}{t})}\big) \ ,$$

where $0 \le \varepsilon \le 1 - l_S(f)$.

Proof. Straightforward from Proposition 5. □

In a second time, since

$$\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}_{\mathfrak{u}}(f, K_{\mathfrak{u}}, A(\boldsymbol{\pi}))\Big] = \sum_{\mathbf{k}\in K_{\mathfrak{u}}}\mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}\big(f, A(\boldsymbol{\pi})\big)\big|^2\Big]$$

the analysis of the bias of the parts of variance estimates rests on the following result

Proposition 6. *Let A be a defect-free orthogonal array in dimension d with parameters q, t and λ in $\mathbb{N}^*$ with $t < d$. Let $\mathfrak{u}$ be a non-empty subset of $\{1,\dots,d\}$ and $\mathbf{k} \in \mathbb{Z}^*_{\mathfrak{u}}$. If there exists $\alpha > 2t+1$ such that f and f^2 are in $\mathcal{H}_\alpha$, we have*

$$\mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big|^2\Big] = \frac{n-1}{n}|\mathrm{c}_{\mathbf{k}}(f)|^2 + \frac{1}{n}\big(\mathrm{V}(f) + \mathrm{c}_{\mathbf{0}}(f)^2 - R_1 - R_2\big) + O\big(n^{-(1+\frac{1}{t})}\big)$$

where

$$R_1(q,t,\lambda,\mathbf{k}) = \sum_{\substack{1\le|\mathfrak{v}|\le t\\ \mathfrak{u}\cap\mathfrak{v}=\emptyset}} \sum_{\mathbf{h}\in\mathbb{Z}^*_{\mathfrak{v}}(q)} \left|\mathrm{c}_{\mathbf{k}+\mathbf{h}}(f)\right|^2$$

consists of terms of order strictly higher than $|\mathfrak{u}|$, *and*

$$R_2(q,t,\lambda,\mathbf{k}) = \sum_{\substack{1\le|\mathfrak{v}|\le t\\ \mathfrak{u}\cap\mathfrak{v}\neq\emptyset}} \sum_{\mathfrak{v}'\subseteq\mathfrak{v}} (-1)^{|\mathfrak{v}|-|\mathfrak{v}'|} \sum_{\mathfrak{v}''\subseteq\mathfrak{v}'} \sum_{\mathbf{h}\in\mathbb{Z}^*_{\mathfrak{v}''}(q)} \left|\mathrm{c}_{\mathbf{k}_{\mathfrak{v}'}+\mathbf{h}}(f)\right|^2$$

where $(\mathbf{k}_{\mathfrak{v}'})_i = 0$ *if* $i\in\mathfrak{v}'$, *and* $(\mathbf{k}_{\mathfrak{v}'})_i = k_i$ *otherwise.*

Proof. See Appendix A.7. □

We conclude that estimators in RBD are asymptotically unbiased in unweighted Korobov spaces since

$$\begin{aligned}
\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}(f,A(\boldsymbol{\pi}))\Big] &= V(f) + \frac{B_1}{n} + o(n^{-1})\\
\mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f,A(\boldsymbol{\pi}))\big|^2\Big] &= |\mathrm{c}_{\mathbf{k}}|^2 + \frac{B_2}{n} + o(n^{-1})
\end{aligned}$$

where $B_1 \le \mathrm{V}(f)$ and $B_2 \le \mathrm{V}(f) + \mathrm{c}_{\mathbf{0}}(f)^2$, and more generally

$$\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}_{\mathfrak{u}}(f,K_{\mathfrak{u}},A(\boldsymbol{\pi}))\Big] = V_{\mathfrak{u}}(f) + \frac{B_3}{n} + \varepsilon_{trunc}(K_{\mathfrak{u}}) + o(n^{-1})$$

where $B_3 \le |K_{\mathfrak{u}}|(\mathrm{V}(f) + \mathrm{c}_{\mathbf{0}}(f)^2)$ and

$$\varepsilon_{trunc}(K_{\mathfrak{u}}) = \sum_{\mathbf{k}\in\mathbb{Z}^*_{\mathfrak{u}}\setminus K_{\mathfrak{u}}} |\mathrm{c}_{\mathbf{k}}(f)|^2$$

is for instance of order $O(M^{|\mathfrak{u}|-\alpha})$ if $K_{\mathfrak{u}} = \mathbb{Z}^*_{\mathfrak{u}}(M)$. Nevertheless, we propose a correction method to reduce a part of these biases.

4.2.3 Application to bias correction

We do not propose any bias correction for the variance estimates since in practice the bias of the latter is generally negligible. So, we are only interested in the bias of the parts of variance estimates

$$\begin{aligned}
\widehat{\mathrm{V}}_{\mathfrak{u}}(M) &= \widehat{\mathrm{V}}_{\mathfrak{u}}\big(f,\mathbb{Z}^*_{\mathfrak{u}}(M),A(\boldsymbol{\pi})\big) \quad , \; 1\le M\le q\\
\widehat{\mathrm{V}}_{\mathfrak{u}}(K_{\mathfrak{u}}) &= \widehat{\mathrm{V}}_{\mathfrak{u}}\big(f,K_{\mathfrak{u}},A(\boldsymbol{\pi})\big) \qquad\quad , \; K_{\mathfrak{u}}\subseteq\mathbb{Z}^*_{\mathfrak{u}}(q)
\end{aligned}$$

under the assumptions of Proposition 6. In practice, the truncation parameter M, as well as the term $|K_{\mathfrak{u}}|^{1/|\mathfrak{u}|}$, is of order 5 or higher, and is generally less than 15. For convenience, we now simply denote $R_1(\mathbf{k}) = R_1(q,t,\lambda,\mathbf{k})$ and $R_1(K) = \sum_{\mathbf{k}\in K} R_1(q,t,\lambda,\mathbf{k})$.

Example 1 $(t = 1,\ |\mathfrak{u}| = 1)$ Let $1 \le i \le d$ and $\mathbf{k} \in \mathbb{Z}^*_{\{i\}}$, we have

$$\mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big|^2\Big] = |\mathrm{c}_{\mathbf{k}}(f)|^2 + \frac{1}{n}\mathrm{V}_{\sim i}(f) - \frac{1}{n}R_1(\mathbf{k}) + O\big(n^{-2}\big) \tag{28}$$

where $\mathrm{V}_{\sim i}(f) = \mathrm{V}(f) - \mathrm{V}_i(f)$. Consequently, for any integer $M \le q$, the estimator $\widehat{\mathrm{V}}_i(M)$ satisfies

$$\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}_i(M)\Big] = \frac{n-(M-1)}{n}\mathrm{V}_i(f) + \frac{M-1}{n}\mathrm{V}(f) - \frac{1}{n}R_1\big(\mathbb{Z}^*_{\{i\}}(M)\big) + O(M^{1-\alpha}) + (M-1)O\big(n^{-2}\big)$$

and should be corrected as follows

$$\widehat{\mathrm{V}}^c_i(M) = \frac{n}{n-(M-1)}\widehat{\mathrm{V}}_i(M) - \frac{M-1}{n-(M-1)}\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big).$$

Proceeding in this way, the remaining bias is

$$\frac{1}{n-(M-1)}\Big[nO\big(M^{1-\alpha}\big) + (M-1)O\big(n^{-1}\big) - R_1\big(\mathbb{Z}^*_i(M)\big)\Big]$$

where $R_1(\mathbb{Z}^*_i(M)) \le \sum_{j\neq i}\mathrm{V}_{ij}(f)$. Note that (28) was partially guessed by Xu & Gertner in [44] (see (44) in their paper) and the bias correction is the same as suggested by Plischke in [27] and proposed by Tissot & Prieur in [40]. More generally, let $K_{\{i\}}$ be a finite subset of $\mathbb{Z}^*_{\{i\}}(q)$; the estimator $\widehat{\mathrm{V}}_i(K_{\{i\}})$ should be corrected as follows

$$\widehat{\mathrm{V}}^c_i(K_{\{i\}}) = \frac{n}{n-|K_{\{i\}}|}\widehat{\mathrm{V}}_i(K_{\{i\}}) - \frac{|K_{\{i\}}|}{n-|K_{\{i\}}|}\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big).$$

Example 2 $(t = 1,\ |\mathfrak{u}| = 2)$ This example may be considered as a problematic case since $|\mathfrak{u}| > t$. Let $1 \le i < j \le d$ and $\mathbf{k} \in \mathbb{Z}^*_{\{i,j\}}$, we have

$$\mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big|^2\Big] = \frac{n+1}{n}|\mathrm{c}_{\mathbf{k}}(f)|^2 + \frac{1}{n}\big(\mathrm{V}(f) + \mathrm{c}_{\mathbf{0}}(f)^2\big) + O\big(n^{-2}\big) - \frac{1}{n}\big(R_1(\mathbf{k}) + R_3(\mathbf{k})\big)$$

where

$$R_3(\mathbf{k}) = \frac{1}{n}\Big(|\mathrm{c}_{\mathbf{k}_{\{i\}}}(f)|^2 + |\mathrm{c}_{\mathbf{k}_{\{j\}}}(f)|^2 + \sum_{\mathbf{h}\in\mathbb{Z}^*_{\{i\}}(q)}|\mathrm{c}_{\mathbf{k}_{\{i\}}+\mathbf{h}}(f)|^2 + \sum_{\mathbf{h}\in\mathbb{Z}^*_{\{j\}}(q)}|\mathrm{c}_{\mathbf{k}_{\{j\}}+\mathbf{h}}(f)|^2\Big).$$

Then for any integer $M \le q$, the estimator $\widehat{\mathrm{V}}_{ij}(M)$ satisfies

$$\begin{aligned}\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}_{ij}(M)\Big] &= \frac{n+1}{n}\mathrm{V}_{ij}(f) + \frac{(M-1)^2}{n}\big(\mathrm{V}(f) + \mathrm{c}_{\mathbf{0}}(f)^2\big) + O(M^{2-\alpha}) + (M-1)^2O\big(n^{-2}\big)\\ &- \frac{1}{n}\Big(R_1\big(\mathbb{Z}^*_{\{i,j\}}(M)\big) + R_3\big(\mathbb{Z}^*_{\{i,j\}}(M)\big)\Big)\end{aligned}$$

and should be corrected as follows

$$\widehat{\mathrm{V}}^c_{ij}(M) = \frac{n}{n+1}\widehat{\mathrm{V}}_{ij}(M) - \frac{(M-1)^2}{n+1}\Big(\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big) + \widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)^2\Big).$$

Proceeding in this way, the remaining bias is

$$\frac{1}{n+1}\Big[nO\big(M^{2-\alpha}\big)+(M-1)^2O\big(n^{-1}\big)-R_1\big(\mathbb{Z}^*_{\{i,j\}}(M)\big)-R_3\big(\mathbb{Z}^*_{\{i,j\}}(M)\big)\Big]$$

where $R_1(\mathbb{Z}^*_{\{i,j\}}(M))\le\sum_{l\neq i,j}\mathrm{V}_{ijl}(f)$ and $R_3(\mathbb{Z}^*_{\{i,j\}}(M))\le(M-1)(\mathrm{V}_i(f)+\mathrm{V}_j(f)+2\mathrm{V}_{ij}(f))$. More generally, let $K_{\{i,j\}}$ be a finite subset of $\mathbb{Z}^*_{\{i,j\}}(q)$; the estimator $\widehat{\mathrm{V}}_{ij}(K_{\{i,j\}})$ should be corrected as follows

$$\widehat{\mathrm{V}}^c_{ij}(K_{\{i,j\}})=\frac{n}{n+1}\widehat{\mathrm{V}}_{ij}(K_{\{i,j\}})-\frac{|K_{\{i,j\}}|}{n+1}\Big(\widehat{\mathrm{V}}\big(f,A(\boldsymbol{\pi})\big)+\widehat{\mathrm{c}}_{\mathbf{0}}\big(f,A(\boldsymbol{\pi})\big)^2\Big).$$

Example 3 ($t=2$, $|\mathfrak{u}|=1$) Let $1\le i\le d$ and $\mathbf{k}\in\mathbb{Z}^*_{\{i\}}$, we have

$$\mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f,A(\boldsymbol{\pi}))\big|^2\Big]=|\mathrm{c}_{\mathbf{k}}(f)|^2+\frac{1}{n}\mathrm{V}_{\sim II}(f)-\frac{d-1}{n}\mathrm{V}_i(f)-\frac{1}{n}R_1'(\mathbf{k})+O\big(n^{-3/2}\big)$$

where $\mathrm{V}_{\sim II}(f)=\mathrm{V}(f)-\sum_{j=1}^d\mathrm{V}_j(f)-\sum_{\substack{j=1\\ j\neq i}}^d\mathrm{V}_{ij}(f)$ and

$$R_1'(\mathbf{k})=\sum_{\substack{|\mathfrak{v}|=2\\ \mathfrak{u}\cap\mathfrak{v}=\emptyset}}\sum_{\mathbf{h}\in\mathbb{Z}^*_{\mathfrak{v}}(q)}\big|\mathrm{c}_{\mathbf{k}+\mathbf{h}}(f)\big|^2.$$

Consequently, for any integer $M\le q$, the estimator $\widehat{\mathrm{V}}_i(M)$ satisfies

$$\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}_i(M)\Big]=\frac{n-(d-1)(M-1)}{n}\mathrm{V}_i(f)+\frac{M-1}{n}\mathrm{V}_{\sim II}(f)-\frac{1}{n}R_1\big(\mathbb{Z}^*_{\{i\}}(M)\big)\cdots$$
$$+O\big(M^{1-\alpha}\big)+(M-1)O\big(n^{-3/2}\big)$$

where

$$R_1'(\mathbb{Z}^*_{\{i\}}(M))\le\sum_{\substack{j<k\\ j,k\neq i}}\mathrm{V}_{ijk}(f).$$

In this case a bias correction could be performed on the term $\mathrm{V}_{\sim II}(f)$, but this is quite intricate — a linear system inversion is needed and the variance of the corrected estimator could significantly increase — and we prefer to keep the basic estimator without bias correction. Proceeding in this way, the bias is

$$B_i=\lambda\mathrm{V}_i(f)+\frac{\lambda}{d-1}\mathrm{V}_{\sim II}(f)-\frac{\lambda}{(d-1)(M-1)}R_1\big(\mathbb{Z}^*_{\{i\}}(M)\big)+O\big(M^{1-\alpha}\big)+(M-1)O\big(n^{-3/2}\big).$$

where $\lambda=(d-1)(M-1)/n$ should be small in practice. More generally, let $K_{\{i\}}$ be a finite subset of $\mathbb{Z}^*_{\{i\}}(q)$; the estimator $\widehat{\mathrm{V}}_i(K_{\{i\}})$ should be kept without bias correction.

Example 4 **($t=2$, $|\mathfrak{u}|=2$)** Let $1 \le i < j \le d$ and $\mathbf{k} \in \mathbb{Z}^*_{\{i,j\}}$, we have

$$\mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big|^2\Big] = |\mathrm{c}_{\mathbf{k}}(f)|^2 + \frac{1}{n}\mathrm{V}_{\sim ij}(f) - \frac{1}{n}R_1(\mathbf{k}) - \frac{1}{n}R_3(\mathbf{k}) + O\big(n^{-3/2}\big)$$

where $\mathrm{V}_{\sim ij}(f) = \mathrm{V}(f) - \mathrm{V}_i(f) - \mathrm{V}_j(f) - \mathrm{V}_{ij}(f)$, and

$$\begin{aligned} R_3(\mathbf{k}) \;&=\; \sum_{\substack{l=1 \\ l \notin \{i,j\}}}^{d} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\{l\}}(q)} \Big(|\mathrm{c}_{\mathbf{k}_{\{i\}}+\mathbf{h}}(f)|^2 + |\mathrm{c}_{\mathbf{k}_{\{j\}}+\mathbf{h}}(f)|^2 - 2|\mathrm{c}_{\mathbf{k}+\mathbf{h}}(f)|^2 \cdots \\ &\quad + \sum_{\mathbf{h}' \in \mathbb{Z}^*_{\{i\}}(q)} |\mathrm{c}_{\mathbf{k}_{\{i\}}+\mathbf{h}+\mathbf{h}'}(f)|^2 + \sum_{\mathbf{h}' \in \mathbb{Z}^*_{\{j\}}(q)} |\mathrm{c}_{\mathbf{k}_{\{j\}}+\mathbf{h}+\mathbf{h}'}(f)|^2 \Big) \,. \end{aligned}$$

Then for any integer $M \le q$, the estimator $\widehat{\mathrm{V}}_{ij}(M)$ satisfies

$$\begin{aligned} \mathbb{E}_\mu\Big[\widehat{\mathrm{V}}_{ij}(M)\Big] &= \frac{n-(M-1)^2}{n}\mathrm{V}_{ij}(f) + \frac{(M-1)^2}{n}\big(\mathrm{V}(f) - \mathrm{V}_i(f) - \mathrm{V}_j(f)\big) \\ &- \frac{1}{n}R_1\big(\mathbb{Z}^*_{\{i,j\}}(M)\big) - \frac{1}{n}R_3\big(\mathbb{Z}^*_{\{i,j\}}(M)\big) + (M-1)^2 O\big(n^{-3/2}\big) + O(M^{2-\alpha}). \end{aligned}$$

and should be corrected as follows

$$\widehat{\mathrm{V}}^c_{ij}(M) = \frac{1}{n-(M-1)^2}\Big(n\widehat{\mathrm{V}}_{ij}(M) - (M-1)^2\Big(\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big) - \widehat{\mathrm{V}}_i(M) - \widehat{\mathrm{V}}_j(M)\Big)\Big).$$

Proceeding in this way, the remaining bias is

$$\begin{aligned} \frac{1}{n-(M-1)^2}\Big[&- R_1\big(\mathbb{Z}^*_{\{i,j\}}(M)\big) - R_3\big(\mathbb{Z}^*_{\{i,j\}}(M)\big) + (M-1)^2 O\big(n^{-1/2}\big) + nO\big(M^{2-\alpha}\big) \cdots \\ &+ (M-1)^2\big(B_i + B_j\big)\Big] \end{aligned}$$

where

$$\begin{aligned} R_1(\mathbb{Z}^*_{\{i\}}(M)) \;&\le\; \sum_{k \notin \{i,j\}} \mathrm{V}_{ijk}(f) + \sum_{\substack{k<l \\ \{k,l\} \cap \{i,j\} \neq \emptyset}} \mathrm{V}_{ijkl}(f) \\ R_3(\mathbb{Z}^*_{\{i\}}(M)) \;&\le\; \sum_{k \notin \{i,j\}} \Big(2(M-2)\mathrm{V}_{ijk}(f) + (M-1)\mathrm{V}_{ik}(f) + (M-1)\mathrm{V}_{jk}(f) \Big) \end{aligned}$$

and where the B_i's are the remaining bias in Example 3. More generally, let $K_{\{i,j\}}$ be a finite subset of $\mathbb{Z}^*_{\{i,j\}}(q)$; the estimators $\widehat{\mathrm{V}}_{ij}(K_{\{i,j\}})$ should be corrected as follows

$$\widehat{\mathrm{V}}^c_{ij}(K_{\{i,j\}}) = \frac{1}{n-|K_{\{i,j\}}|}\Big(n\widehat{\mathrm{V}}_{ij}(K_{\{i,j\}}) - |K_{\{i,j\}}|\Big(\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big) - \widehat{\mathrm{V}}_i(K_{\{i\}}) - \widehat{\mathrm{V}}_j(K_{\{j\}})\Big)\Big).$$

In the sequel, we denote $\widehat{\mathrm{S}}^c_{\mathfrak{u}}\big(f, K, A(\boldsymbol{\pi})\big)$ the index $\widehat{\mathrm{V}}^c_{\mathfrak{u}}\big(f, K, A(\boldsymbol{\pi})\big)/\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big)$.

5 Numerical illustrations

In this section, we apply the bias correction method of Section 4.2.3. on the first and the second-order sensitivity indices computed with RBD when the model is the Sobol' g-function (see [35])

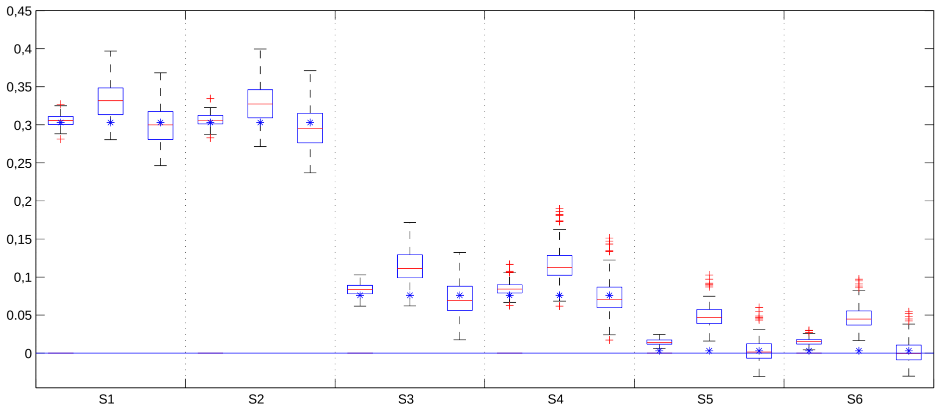
$$f(X_1, \ldots, X_d) = \prod_{i=1}^{d} \frac{|4X_i - 2| + a_i}{1 + a_i}$$

where the a_i's are non-negative parameters and the X_i's are independent random variables uniformly distributed in $[0, 1]$. Note that for any $\mathbf{k} \in \mathbb{Z}^d$

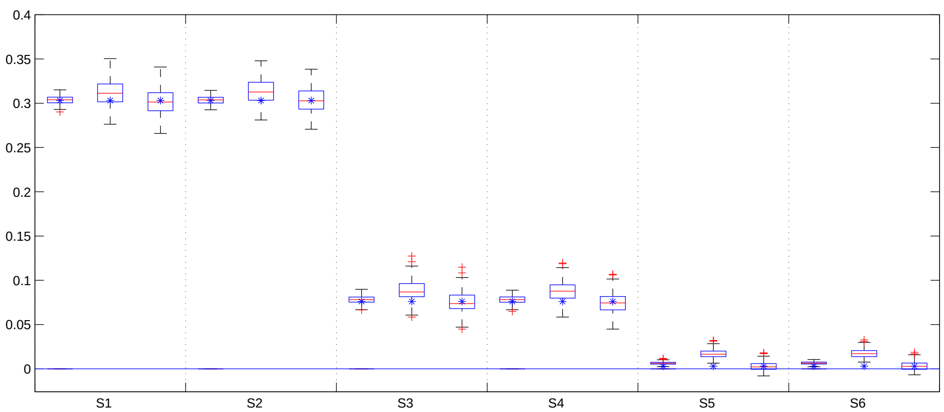
$$\mathrm{c}_{\mathbf{k}}(f) = \begin{cases} 0 & \text{if } \exists i \in \{1, \ldots, d\} \mid k_i \neq 0 \text{ and } k_i \text{ is even} \\[2ex] \dfrac{\displaystyle\prod_{i \mid k_i \neq 0} 4\pi^{-2}(1 + a_i)^{-1}}{\displaystyle\prod_{i \mid k_i \neq 0} k_i^2} & \text{otherwise} \end{cases}$$

We consider a test-case with $d = 6$ and $\mathbf{a} = (0, 0, 1, 1, 9, 9)$. Exact values of the sensitivity indices are known; we have $\mathrm{S}_1(f) = \mathrm{S}_2(f) = 0.303$, $\mathrm{S}_3(f) = \mathrm{S}_4(f) = 0.076$, $\mathrm{S}_{12} = 0.101$,$\mathrm{S}_{13}(f) = \mathrm{S}_{14}(f) = \mathrm{S}_{23}(f) = \mathrm{S}_{24}(f) = 0.025$, $\mathrm{S}_{34} = 0.006$ and the other indices are less than 5.10^{-3}. In each illustration, we show boxplots of 100 estimates computed on a randomized array $A(\boldsymbol{\pi})$ — see Section 4.2.1. — of a certain orthogonal array A. In these boxplots, the red central mark is the median; the box has its lower and upper edges at the 25^{th} percentile q and the 75^{th} percentile Q, respectively; the whiskers extend between $q - 1.5(Q - q)$ and $Q + 1.5(Q - q)$; the red crosses are outliers and blue asterisks are exact values. Two arrays A are tested. The first one, denoted $A_{1,n}$, is an orthogonal array with index unity, strength 1 and q levels — and then $n = q$ —; it corresponds with the classic RBD method and its construction is obvious. The second one, denoted $A_{2,n}$ is an orthogonal array with index unity, strength 2 and q levels, where q is a prime — and then $n = q^2$. This array is obtained by using Bush's construction (see [4]).

Figure 3 shows boxplots of the first-order sensitivity indices estimates when the orthogonal array A is $A_{1,529}$, $A_{2,529}$, $A_{1,1681}$ and $A_{2,1681}$, with and without bias correction. We see obviously that A_2 leads to better estimates than A_1 in term of variance. We also notice that the bias correction perfomed, when A_1 is used, is efficient; and the estimates, when A_2 is used, are almost without any bias. Figure 4 shows boxplots of six of the fifteen second-order sensitivity estimates when the orthogonal array A is $A_{1,1681}$, $A_{2,1681}$, $A_{1,3481}$ and $A_{2,3481}$, with and without bias correction. One more time, A_2 leads to better estimates than A_1 in term of variance, and the bias correction methods perform well.



(a) $n = 529$

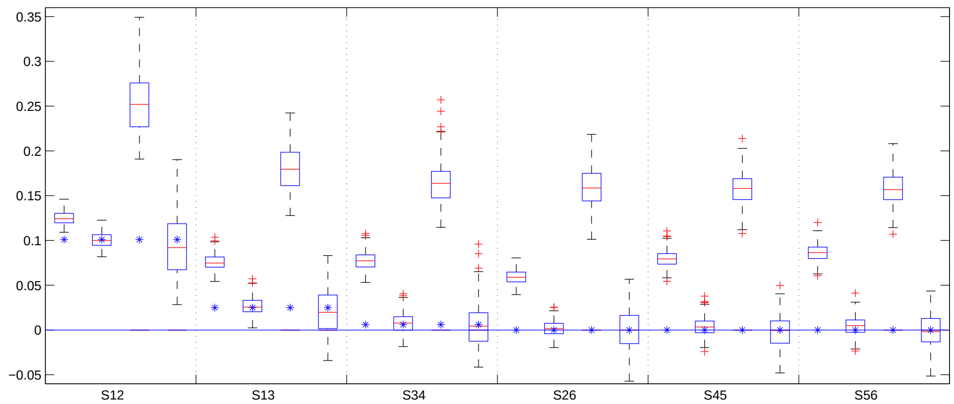


(b) $n = 1681$

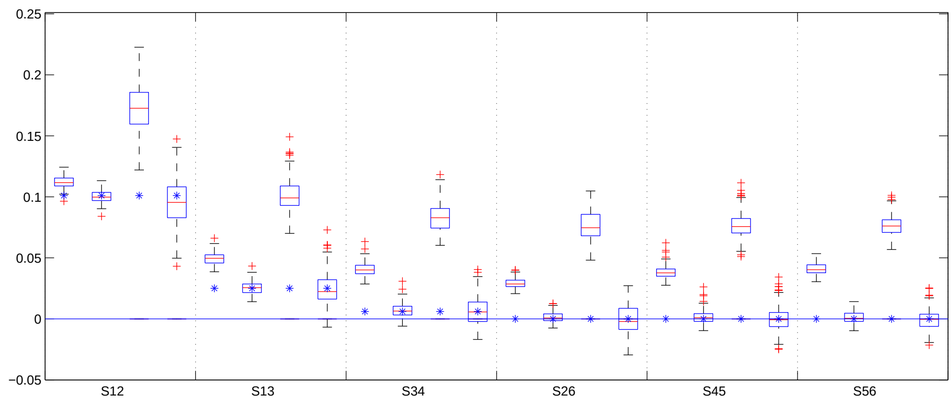
Figure 3: Boxplots of the first-order sensitivity indices estimates. For each sensitivity index, from the left to the right are $\widehat{\mathrm{S}}_i\big(\mathcal{R}_1 f, \mathcal{Z}_{\{i\},12}, A_2(\boldsymbol{\pi})\big)$, $\widehat{\mathrm{S}}_i\big(\mathcal{R}_1 f, \mathcal{Z}_{\{i\},12}, A_1(\boldsymbol{\pi})\big)$, $\widehat{\mathrm{S}}_i^c\big(\mathcal{R}_1 f, \mathcal{Z}_{\{i\},12}, A_1(\boldsymbol{\pi})\big)$, respectively.

6 Conclusions

In this paper we revisited the variance-based sensitivity methods, FAST and RBD, by linking them to commonly used methods in numerical integration field. They are introduced in light of the DFT on finite subgroups of the torus and the use of randomized orthogonal arrays for integration. First we explained the classic FAST in terms of trigonometric interpolation and we introduced a new criterion to choose the set of frequencies free of interferences. We also derived, from the lattice rules theory, explicit rates of convergence for the estimators of the first and second-order partial variances,



(a) $n = 1681$



(b) $n = 3481$

Figure 4: Boxplots of the second-order sensitivity indices estimates. For each sensitivity index, from the left to the right are $\widehat{\mathrm{S}}_{ij}\big(\mathcal{R}_1 f, \mathcal{Z}_{\{i,j\},12}, A_{2,n}(\boldsymbol{\pi})\big)$, $\widehat{\mathrm{S}}^c_{ij}\big(\mathcal{R}_1 f, \mathcal{Z}_{\{i,j\},12}, A_{2,n}(\boldsymbol{\pi})\big)$, $\widehat{\mathrm{S}}_{ij}\big(\mathcal{R}_1 f, \mathcal{Z}_{\{i,j\},12}, A_{1,n}(\boldsymbol{\pi})\big)$, $\widehat{\mathrm{S}}^c_{ij}\big(\mathcal{R}_1 f, \mathcal{Z}_{\{i,j\},12}, A_{1,n}(\boldsymbol{\pi})\big)$, respectively.

and the total variance. In a second time, we explained the classic RBD in terms of integration on a randomized orthogonal array with strength 1, and naturally generalized this method to any orthogonal array. We then studied the well-known issue due to the bias and proposed a correction method in the most common cases. Further work will consist in investigating the variance of the estimators in RBD in order to propose a bias-variance trade-off. As far as we know, apart from the application of shrinkage due to Tarantola & Koda [39], this issue related to the variance is not studied much. It will also consists in applying the FAST method by following Proposition 4 and employing embedded lattice rules (see [6]).

Acknowledgments

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A Proofs of the propositions

A.1 Proof of Proposition 2

On the one hand, noting that for all $x \in \mathbb{R}$,

$$\arcsin\big(\sin(x)\big) = \arcsin\Big(\sin\Big(2\pi\Big\{\frac{x}{2\pi}\Big\}\Big)\Big) = \begin{cases} 2\pi\{\frac{x}{2\pi}\} & \text{if } 0 \le \{\frac{x}{2\pi}\} < \frac{1}{4} \\ \pi - 2\pi\{\frac{x}{2\pi}\} & \text{if } \frac{1}{4} \le \{\frac{x}{2\pi}\} < \frac{3}{4} \\ 2\pi\{\frac{x}{2\pi}\} - 2\pi & \text{otherwise} \end{cases} \tag{A.1}$$

we get that for any $i \in \{1, \dots d\}$ and $j \in \{0, \dots, n-1\}$,

$$x_i^*\Big(\frac{j}{n}\Big) = \frac{1}{\pi}\arcsin\Big(\sin\Big(2\pi\omega_i\frac{j}{n} + \varphi_i\Big)\Big) + \frac{1}{2} = r_1 \circ t_{\varphi_i}\Big(\Big\{\frac{j}{n}\omega_i\Big\}\Big).$$

Thus we have

$$f \circ \mathbf{x}^*\Big(\frac{j}{n}\Big) = (\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1)f\Big(\Big\{\frac{j}{n}\omega_1\Big\}, \dots, \Big\{\frac{j}{n}\omega_d\Big\}\Big), \tag{A.2}$$

and we easily deduce that for all $\mathbf{k} \in \mathbb{Z}^d$,

$$\big|\widehat{\mathrm{c}}_{\mathbf{k}\cdot\boldsymbol{\omega}}(f \circ \mathbf{x}^*)\big| = \big|\widehat{\mathrm{c}}_{\mathbf{k}}\big((\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1)f, G(\boldsymbol{\omega})\big)\big|.$$

Finally we obtain that for any non-empty set $\mathfrak{u} \subseteq \{1, \dots, d\}$ and any finite set $K_\mathfrak{u} \subseteq \mathbb{Z}_\mathfrak{u}^*$

$$\widehat{\mathrm{V}}_\mathfrak{u}^{\mathrm{FAST}}(f, K_\mathfrak{u}, \mathbf{x}^*) = \widehat{\mathrm{V}}_\mathfrak{u}\big((\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1)f, K_\mathfrak{u}, G(\boldsymbol{\omega})\big). \tag{A.3}$$

Recalling that $\widehat{\mathrm{V}}^{\mathrm{FAST}}(f, \mathbf{x}^*) = \widehat{\mathrm{V}}(f, \{\mathbf{x}^*(\frac{j}{n})\}_{j=0..n-1})$, (A.2) obviously leads to

$$\widehat{\mathrm{V}}^{\mathrm{FAST}}(f, \mathbf{x}^*) = \widehat{\mathrm{V}}\big((\mathcal{T}_{\boldsymbol{\varphi}} \circ \mathcal{R}_1)f, G(\boldsymbol{\omega})\big). \tag{A.4}$$

We conclude to (18) by combining (A.3) and (A.4).

On the other hand, we also deduce from (A.1) that for any $i \in \{1, \dots d\}$ and $j \in \{0, \dots, n-1\}$,

$$x_i^\times\Big(\frac{j}{n}\Big) = \frac{1}{\pi}\arcsin\Big(\sin\Big(2\pi\omega\frac{\sigma_i(j)}{n}\Big)\Big) + \frac{1}{2} = r_\omega \circ t_{\frac{(1-\omega)\pi}{2\omega}}\Big(\frac{\sigma_i(j)}{n}\Big). \tag{A.5}$$

Thus we have

$$f \circ \mathbf{x}^{\times}\Big(\frac{j}{n}\Big) = (\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_{\omega}) f\Big(\frac{\sigma_1(j)}{n}, \dots, \frac{\sigma_d(j)}{n}\Big), \tag{A.6}$$

and we easily deduce that for all $i \in \{1, \dots, d\}$ and $k_i \in \mathbb{Z}$,

$$\widehat{\mathrm{c}}_{k_i\omega}(f \circ \mathbf{x}^{\times,i}) = \widehat{\mathrm{c}}_{(0,\dots,0,k_i\omega,0,\dots,0)}\big((\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_{\omega}) f, A(\boldsymbol{\sigma})\big). \tag{A.7}$$

Finally we obtain that for any non-empty $i \in \{1, \dots, d\}$ and any finite set $K_{\{i\}} \subseteq \mathbb{Z}^*_{\{i\}}$

$$\widehat{\mathrm{V}}_i^{\mathrm{RBD}}(f, K_{\{i\}}, \mathbf{x}^{\times}) = \widehat{\mathrm{V}}_i\big((\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_{\omega}) f, \omega K_{\{i\}}, A(\boldsymbol{\sigma})\big). \tag{A.8}$$

Recalling that $\widehat{\mathrm{V}}^{\mathrm{RBD}}(f, \mathbf{x}^{\times}) = \widehat{\mathrm{V}}(f, \{\mathbf{x}^{\times}(\frac{j}{n})\}_{j=0..n-1})$, (A.6) obviously leads to

$$\widehat{\mathrm{V}}^{\mathrm{RBD}}(f, \mathbf{x}^{\times}) = \widehat{\mathrm{V}}\big((\mathcal{T}_{\tilde{\boldsymbol{\omega}}} \circ \mathcal{R}_{\omega}) f, A(\boldsymbol{\sigma})\big). \tag{A.9}$$

We conclude to (19) by combining (A.8) and (A.9).

A.2 Further issue: influence of the parameter ω in the classic RBD

In the proof of Proposition 2, it is easy to show that Eqs. (A.5) to (A.9) can be successively replaced by

$$\begin{aligned}
x_i^{\times}\Big(\frac{j}{n}\Big) &= r_1\Big(\Big\{\omega\frac{\sigma_i(j)}{n}\Big\}\Big) \\
f \circ \mathbf{x}^{\times}\Big(\frac{j}{n}\Big) &= \mathcal{R}_1 f\Big(\Big\{\omega\frac{\sigma_1(j)}{n}\Big\}, \dots, \Big\{\omega\frac{\sigma_d(j)}{n}\Big\}\Big) \\
\widehat{\mathrm{c}}_{k_i\omega}(f \circ \mathbf{x}^{\times,i}) &= \widehat{\mathrm{c}}_{(0,\dots,0,k_i,0,\dots,0)}\big(\mathcal{R}_1 f, \{\omega A(\boldsymbol{\sigma})\}\big) \\
\widehat{\mathrm{V}}_i^{\mathrm{RBD}}(f, K_{\{i\}}, \mathbf{x}^{\times}) &= \widehat{\mathrm{V}}_i\big(\mathcal{R}_1 f, K_{\{i\}}, \{\omega A(\boldsymbol{\sigma})\}\big)
\end{aligned}$$

and

$$\widehat{\mathrm{V}}^{\mathrm{RBD}}(f, \mathbf{x}^{\times}) = \widehat{\mathrm{V}}\big(\mathcal{R}_1 f, \{\omega A(\boldsymbol{\sigma})\}\big),$$

where

$$\{\omega A(\boldsymbol{\sigma})\} = \Big\{\Big(\Big\{\omega\frac{\sigma_1(j)}{n}\Big\}, \dots, \Big\{\omega\frac{\sigma_d(j)}{n}\Big\}\Big),\ j \in \{0, \dots, n-1\}\Big\}.$$

Consequently, (19) can be replaced by

$$\widehat{\mathrm{S}}_i^{\mathrm{RBD}}(f, K_{\{i\}}, \mathbf{x}^{\times}) = \widehat{\mathrm{S}}_i\big(\mathcal{R}_1 f, K_{\{i\}}, \{\omega A(\boldsymbol{\sigma})\}\big), \tag{A.10}$$

and it means that ω has an influence on the estimator through the orthogonal array on which the function $\mathcal{R}_1 f$ is evaluated.

Now following the Definition 2 in Section 4.2., note that if A is an orthogonal array with q levels $\{0, \frac{1}{q}, \ldots, \frac{q-1}{q}\}$, strength t and index λ — and denote $n = \lambda q^t$ its cardinal —, then for any $p \in \mathbb{N}^*$, $\{pA\}$ is an orthogonal array with $q' = q/gcd(p,q)$ levels $\{0, \frac{1}{q'}, \ldots, \frac{q'-1}{q'}\}$, strength t' larger or equal to t, and index $\lambda' = n/(q't')$. Indeed, consider $\{0, \frac{1}{q}, \ldots, \frac{q-1}{q}\}$ as the cyclic group $\mathbb{Z}/q\mathbb{Z}$ and note that the homomorphism

$$\begin{array}{rccc} \Phi: & \mathbb{Z}/q\mathbb{Z} & \longrightarrow & \mathbb{Z}/q\mathbb{Z} \\ & \overline{z} & \longmapsto & \overline{pz} \end{array}$$

is surjective on $\mathbb{Z}/q'\mathbb{Z}$, where $q' = q/gcd(p,q)$. Consequently, it is easy to deduce that $\{pA\}$ has q' levels and has at least strength t.

As a consequence, in the classic RBD, if ω is relatively prime with the number of levels of the orthogonal array $A(\boldsymbol{\sigma})$ — recall that it is $|A(\boldsymbol{\sigma})|/2$ if $A(\boldsymbol{\sigma})$ is even and $|A(\boldsymbol{\sigma})|$ otherwise —, then the method is exactly equivalent to the basic one with $\omega = 1$. On the contrary, if they are not relatively prime, the orthogonal array on which $\mathcal{R}_1 f$ is evaluated has fewer levels and at least the same strength. Moreover in this case, the orthogonal array could be not simple, i.e. its points are not distinct. Thus the estimator (A.10) has potentially a larger bias and a larger variance.

A.3 Proof of Lemma 1

Let $X_1, \ldots, X_d$ be d independent random variables uniformly distributed on $[0,1]$ and denote $f_{\mathfrak{u}}(X_i, i \in \mathfrak{u})$, $\mathfrak{u} \subseteq \{1, \ldots d\}$ the Hoeffding decomposition of $f(\mathbf{X})$. We first prove the result for the linear operator $\mathcal{R}_1$. Let s be a positive integer and $\mathcal{Q}^s$ be the set of the subset Q of $[0,1[^s$ of the form $\mathrm{Q} = [q_1, q_1 + \frac{1}{2}[\times \cdots \times [q_s, q_s + \frac{1}{2}[$ where $q_i \in \{0, \frac{1}{2}\}$. Note that, since the Lebesgue measure is isometry-invariant, we have for any $\mathrm{Q} \in \mathcal{Q}^s$ and any function $g \in L^2([0,1]^s)$,

$$\int_{\mathrm{Q}} \mathcal{R}_1 g(\mathbf{x}) d\mathbf{x} = \int_{[0,\frac{1}{2}[^s} \mathcal{R}_1 g(\mathbf{x}) d\mathbf{x} \ .$$

Thus it comes

$$\begin{aligned} \int_{[0,1[^s} \mathcal{R}_1 g(\mathbf{x}) d\mathbf{x} &= \sum_{\mathrm{Q} \in \mathcal{Q}^s} \int_{\mathrm{Q}} \mathcal{R}_1 g(\mathbf{x}) d\mathbf{x} \\ &= 2^s \int_{[0,\frac{1}{2}[^s} \mathcal{R}_1 g(\mathbf{x}) d\mathbf{x} \end{aligned}$$

and the definition of $\mathcal{R}_1$ gives

$$\int_{[0,1[^s} \mathcal{R}_1 g(\mathbf{x}) d\mathbf{x} = \int_{[0,1[^s} g(\mathbf{x}) d\mathbf{x} \ . \tag{A.11}$$

Then noting that for all $\mathbf{x} \in [0,1[^d$, $(\mathcal{R}_1 g(\mathbf{x}))^2 = \mathcal{R}_1(g(\mathbf{x}))^2$, we deduce that for all set $\mathfrak{u} \subseteq \{1,\dots,d\}$,

$$\mathrm{Var}\big[\mathcal{R}_1 f_{\mathfrak{u}}(X_i, i \in \mathfrak{u})\big] = \mathrm{Var}\big[f_{\mathfrak{u}}(X_i, i \in \mathfrak{u})\big]. \tag{A.12}$$

We also deduce from (A.11) that for all set $\mathfrak{u} \subseteq \{1,\dots,d\}$,

$$\forall \beta \subsetneq \mathfrak{u}, \quad \mathbb{E}\big[\mathcal{R}_1 f_{\mathfrak{u}}(X_i, i \in \mathfrak{u}) | X_i, i \in \beta\big] = \mathbb{E}\big[f_{\mathfrak{u}}(X_i, i \in \mathfrak{u}) | X_i, i \in \beta\big] \ ,$$

and then, by the uniqueness of the Hoeffding decomposition and the criterion in (2),

$$\forall \mathfrak{u} \subseteq \{1,\dots,d\}, \quad (\mathcal{R}_1 f)_{\mathfrak{u}} = \mathcal{R}_1 f_{\mathfrak{u}} \ . \tag{A.13}$$

Finally (A.12) and (A.13) lead to the conclusion of Lemma 1 for the linear operator $\mathcal{R}_1$. The proof of Lemma 1 for any $\mathcal{R}_p$ with $p \in \mathbb{N}^*$ and for the $\mathcal{T}_{\boldsymbol{\varphi}}$'s is exactly the same as the previous one. It only sufficies to prove that the property in (A.11) hold for any $\mathcal{R}_p$ and $\mathcal{T}_{\boldsymbol{\varphi}}$. This property for the $\mathcal{T}_{\boldsymbol{\varphi}}$'s is a consequence of the translation-invance of the Lebesgue measure and is omitted here. For the $\mathcal{R}_p$'s, note that for all $x \in [0,1]$, $r_p(x) = r_1(\{px\})$ and deduce that for all $\mathbf{x} \in [0,1]^s$, $\mathcal{R}_p g(\mathbf{x}) = \mathcal{R}_1 g(\{px_1\},\dots,\{px_s\})$. Hence, noting that $\mathcal{R}_p g$ is $\frac{1}{p}$-periodic in each direction, it comes

$$\begin{aligned}
\int_{[0,1[^s} \mathcal{R}_p g(\mathbf{x}) d\mathbf{x} &= p^s \int_{[0,\frac{1}{p}[^s} \mathcal{R}_p g(\mathbf{x}) d\mathbf{x} \\
&= p^s \int_{[0,\frac{1}{p}[^s} \mathcal{R}_1 g(px_1,\dots,px_s) d\mathbf{x} \\
&= \int_{[0,1[^s} g(\mathbf{x}) d\mathbf{x} \ .
\end{aligned}$$

A.4 Proof of (24) in Proposition 3

Let $\sim$ denote the relation such that for all $\mathbf{k}$, and $\mathbf{k}'$ in $\mathbb{Z}^d$,

$$\mathbf{k} \sim \mathbf{k}' \Longleftrightarrow \mathbf{k} - \mathbf{k}' \in G^\perp \ .$$

This is obviously an equivalence relation and its classes are of the form

$$G^\perp_{\mathbf{k}} = \{\mathbf{k} + \mathbf{h}, \ \mathbf{h} \in G^\perp\} \ .$$

Hence we have

$$\sum_{\mathbf{k} \in K} \sum_{\mathbf{h} \in G^\perp} \mathrm{c}_{\mathbf{k}+\mathbf{h}}(f) \exp\big(2i\pi(\mathbf{k}+\mathbf{h}) \cdot \mathbf{x}\big) = \sum_{\mathbf{k} \in K} \sum_{\mathbf{h} \in G^\perp_{\mathbf{k}}} \mathrm{c}_{\mathbf{h}}(f) \exp(2i\pi \mathbf{h} \cdot \mathbf{x})$$

Now, under the assumption that G satisfies the criterion (22), for all $\mathbf{k} \in K$ the classes $G^{\perp}_{\mathbf{k}}$ are distinct. Moreover, it can be shown that

$$\mathbb{Z}^d / G^{\perp} \simeq G^*$$

where G^* is the dual group of G (see e.g. Paragraph 2.1.2. in [28]) and as a consequence, the number of classes — which is equal to the cardinal of the quotient $\mathbb{Z}^d/G^{\perp}$ — is equal to $|G^*| = |G| = n$. Thus we have

$$\bigsqcup_{\mathbf{k} \in K} G^{\perp}_{\mathbf{k}} = \mathbb{Z}^d$$

and we conclude that

$$\sum_{\mathbf{k} \in K} \sum_{\mathbf{h} \in G^{\perp}} \mathrm{c}_{\mathbf{k}+\mathbf{h}}(f) \exp\big(2i\pi(\mathbf{k}+\mathbf{h}) \cdot \mathbf{x}\big) = \sum_{\mathbf{k} \in \mathbb{Z}^d} \mathrm{c}_{\mathbf{k}}(f) \exp(2i\pi \mathbf{k} \cdot \mathbf{x}) \ .$$

A.5 Proof of Proposition 4

For convenience we now denote $B(\alpha) = B(\alpha, n, d, \boldsymbol{\gamma})$.

First for any $\mathbf{k} \in \mathbb{Z}^d$ and $f \in \mathcal{H}_{\alpha,\boldsymbol{\gamma}}$, denote $f_{\mathbf{k}} : \mathbf{x} \mapsto f(\mathbf{x})\exp(-2i\pi\mathbf{k}\cdot\mathbf{x})$ and note that $f_{\mathbf{k}} \in \mathcal{H}_{\alpha,\boldsymbol{\gamma}}$, $\mathrm{c}_{\mathbf{0}}(f_{\mathbf{k}}) = \mathrm{c}_{\mathbf{k}}(f)$ and $\widehat{\mathrm{c}}_{\mathbf{0}}(f_{\mathbf{k}}, G) = \widehat{\mathrm{c}}_{\mathbf{k}}(f, G)$. Now we have

$$\begin{aligned}
\big||\widehat{\mathrm{c}}_{\mathbf{k}}(f,G)|^2 - |\mathrm{c}_{\mathbf{k}}(f)|^2\big| &= \big|\big(\widehat{\mathrm{c}}_{\mathbf{k}}(f,G) - \mathrm{c}_{\mathbf{k}}(f)\big)\overline{\widehat{\mathrm{c}}_{\mathbf{k}}(f,G)} - \mathrm{c}_{\mathbf{k}}(f)\big(\overline{\mathrm{c}_{\mathbf{k}}(f)} - \overline{\widehat{\mathrm{c}}_{\mathbf{k}}(f,G)}\big)\big| \\
&\leq \big|\widehat{\mathrm{c}}_{\mathbf{k}}(f,G) - \mathrm{c}_{\mathbf{k}}(f)\big| \cdot \big|\overline{\widehat{\mathrm{c}}_{\mathbf{k}}(f,G)}\big| + \big|\mathrm{c}_{\mathbf{k}}(f)\big| \cdot \big|\overline{\mathrm{c}_{\mathbf{k}}(f)} - \overline{\widehat{\mathrm{c}}_{\mathbf{k}}(f,G)}\big| \\
&\leq ||f_{\mathbf{k}}||_{\mathcal{H}_{\alpha,\boldsymbol{\gamma}}} B(\alpha)\big(2|\mathrm{c}_{\mathbf{k}}(f)| + ||f_{\mathbf{k}}||_{\mathcal{H}_{\alpha,\boldsymbol{\gamma}}} B(\alpha)\big) \ . \qquad \text{(A.14)}
\end{aligned}$$

In particular, for $\mathbf{k} = \mathbf{0}$, it comes

$$\big||\widehat{\mathrm{c}}_{\mathbf{0}}(f,G)|^2 - |\mathrm{c}_{\mathbf{0}}(f)|^2\big| \leq ||f||^2_{\mathcal{H}_{\alpha,\boldsymbol{\gamma}}} B(\alpha)\big(2 + B(\alpha)\big) \ . \qquad \text{(A.15)}$$

We now prove the two items of Proposition 4. For the first one, Note that

$$\begin{aligned}
\big|\widehat{\mathrm{V}}(f,G) - \mathrm{V}(f)\big| &= \left|\frac{1}{n}\sum_{g \in G} f^2(g) - |\widehat{\mathrm{c}}_{\mathbf{0}}(f,G)|^2 - \int_{[0,1]^d} f^2(\mathbf{x}) d\mathbf{x} + |\mathrm{c}_{\mathbf{0}}(f)|^2\right| \\
&\leq \big||\widehat{\mathrm{c}}_{\mathbf{0}}(f^2,G)| - |\mathrm{c}_{\mathbf{0}}(f^2)|\big| + \big||\widehat{\mathrm{c}}_{\mathbf{0}}(f,G)|^2 - |\mathrm{c}_{\mathbf{0}}(f)|^2\big|
\end{aligned}$$

and the conclusion follows from (A.15). For the second item, (A.14) gives

$$\big|\widehat{\mathrm{V}}_{\mathbf{u}}(f, K_{\mathbf{u}}, G) - \mathrm{V}_{\mathbf{u}}(f)\big| = \left| \sum_{\mathbf{k} \in \mathbb{Z}^*_{\mathbf{u}} \setminus K_{\mathbf{u}}} |\mathrm{c}_{\mathbf{k}}(f)|^2 - \sum_{\mathbf{k} \in K_{\mathbf{u}}} \Big(|\mathrm{c}_{\mathbf{k}}(f)|^2 - |\widehat{\mathrm{c}}_{\mathbf{k}}(f,G)|^2\Big)\right|$$

$$\leq \sum_{\mathbf{k}\in\mathbb{Z}_{\mathfrak{u}}^*\setminus K_{\mathfrak{u}}} \frac{||f||^2_{\mathcal{H}_{\alpha,\gamma}}}{r(\mathbf{k},\alpha,\boldsymbol{\gamma})} + B(\alpha)^2 \sum_{\mathbf{k}\in K_{\mathfrak{u}}} ||f_{\mathbf{k}}||^2_{\mathcal{H}_{\alpha,\gamma}} + 2B(\alpha) \sum_{\mathbf{k}\in K_{\mathfrak{u}}} |\mathrm{c}_{\mathbf{k}}(f)| \, ||f_{\mathbf{k}}||_{\mathcal{H}_{\alpha,\gamma}}, \tag{A.16}$$

and the proof is then divided into two parts:

First part. In the second term in the right-hand side of (A.16), let $r(\mathbf{0},\alpha,\boldsymbol{\gamma}) = 1$ and note that

$$||f_{\mathbf{k}}||^2_{\mathcal{H}_{\alpha,\gamma}} = \sum_{\substack{\mathbf{h}\in\mathbb{Z}^d \\ \gamma_{\mathfrak{u}_{\mathbf{h}}}\neq 0}} r(\mathbf{h},\alpha,\boldsymbol{\gamma})|\mathrm{c}_{\mathbf{h}}(f_{\mathbf{k}})|^2 = \sum_{\substack{\mathbf{h}\in\mathbb{Z}^d \\ \gamma_{\mathfrak{u}_{\mathbf{h}}}\neq 0}} \frac{r(\mathbf{h},\alpha,\boldsymbol{\gamma})}{r(\mathbf{h}+\mathbf{k},\alpha,\boldsymbol{\gamma})} r(\mathbf{h}+\mathbf{k},\alpha,\boldsymbol{\gamma})|\mathrm{c}_{\mathbf{h}+\mathbf{k}}(f)|^2 \; .$$

Then denoting $\gamma_{frac} = \max_{\mathfrak{u},\mathfrak{v}\subset\{1,\ldots,d\},\gamma_{\mathfrak{v}}\neq 0} \gamma_{\mathfrak{u}}/\gamma_{\mathfrak{v}}$, for any $\mathbf{k}\in K_{\mathfrak{u}}$,

$$\frac{r(\mathbf{h},\alpha,\boldsymbol{\gamma})}{r(\mathbf{h}+\mathbf{k},\alpha,\boldsymbol{\gamma})} \leq \gamma_{frac} \prod_{i\in\mathfrak{u}} (|k_i|+1)^{\alpha} \tag{A.17}$$

and thus

$$||f_{\mathbf{k}}||_{\mathcal{H}_{\alpha,\gamma}} \leq \gamma_{frac} \prod_{i\in\mathfrak{u}} (|k_i|+1)^{\alpha/2} ||f||_{\mathcal{H}_{\alpha,\gamma}} \; .$$

To prove (A.17), note that

$$\frac{r(\mathbf{h},\alpha,\boldsymbol{\gamma})}{r(\mathbf{h}+\mathbf{k},\alpha,\boldsymbol{\gamma})} = \gamma_{frac} \prod_{i\in\mathfrak{u}} \left(\frac{\max(1,|h_i|)}{\max(1,|h_i+k_i|)} \right)^{\alpha}$$

and prove that for any $h,\ k\in\mathbb{Z}$, we have

$$\frac{\max(1,|h|)}{\max(1,|h+k|)} \leq |k|+1 \; . \tag{A.18}$$

Indeed, it is obvious if $h=0$ or $h=-k$; otherwise,

$$\frac{\max(1,|h|)}{\max(1,|h+k|)} = \frac{|h|}{|h+k|} \; .$$

At last (A.18) is still obvious if h and k have same sign and otherwise,

if $|h| > |k|$ then $|h/(k+h)| = |h|/(|h|-|k|)$ decreases with respect to $|h|$, so $|h/(k+h)| \leq |k|+1$

if if $|h| < [k|$ then $|h/(k+h)| = |h|/(|k|-|h|)$ increases with respect to $|h|$, so $|h/(k+h)| \leq |k|-1$.

Second part. In the first term in the right-hand side of (A.16), denote $K^c_{\mathfrak{u}+} = (\mathbb{Z}^*_{\mathfrak{u}} \setminus K_{\mathfrak{u}}) \cap \mathbb{Z}^d_+$, $I_{\mathfrak{u}} = [1, \beta_{\mathfrak{u}}^{1/|\mathfrak{u}|}] \cap \mathbb{Z}$. Then for any set $\mathfrak{v} \subsetneq \mathfrak{u}$, define

$$Q_{\mathfrak{u},\mathfrak{v}} = \left\{ \mathbf{k}\in K^c_{\mathfrak{u}+},\ \forall i\in\mathfrak{v},\ k_i\in I_{\mathfrak{u}} \ \text{ and } \ \forall i\in\mathfrak{u}\setminus\mathfrak{v},\ k_i\notin I_{\mathfrak{u}} \right\}$$

and note that

$$K^c_{\mathfrak{u}+} = \bigsqcup_{\mathfrak{v}\subsetneq \mathfrak{u}} Q_{\mathfrak{u},\mathfrak{v}}.$$

Hence denoting $\gamma_{max} = \max_{\mathfrak{u}\subset\{1,\ldots,d\}} \gamma_{\mathfrak{u}}$, it comes

$$\begin{aligned}
\sum_{\mathbf{k}\in\mathbb{Z}^*_{\mathfrak{u}}\setminus K_{\mathfrak{u}}} \frac{1}{r(\mathbf{k},\alpha,\boldsymbol{\gamma})} &\leq 2^{|\mathfrak{u}|}\gamma_{max} \sum_{\mathbf{k}\in K^c_{\mathfrak{u}+}} \prod_{i\in\mathfrak{u}} k_i^{-\alpha} \\
&\leq 2^{|\mathfrak{u}|}\gamma_{max} \sum_{\mathfrak{v}\subsetneq\mathfrak{u}} \Bigg(\sum_{\mathbf{k}\in Q_{\mathfrak{u},\mathfrak{v}}} \prod_{i\in\mathfrak{u}} k_i^{-\alpha} \Bigg)
\end{aligned}$$

and it leads to the proof of (26) and (27). If $\mathfrak{u} = \{i\}$,the proof is easy since we have

$$\begin{aligned}
\sum_{\mathbf{k}\in Q_{\{i\},\emptyset}} k_i^{-\alpha} &= \sum_{k=\lfloor\beta_{\{i\}}+1\rfloor}^{+\infty} k^{-\alpha} \\
&= \sum_{j=0}^{\lfloor\beta_{\{i\}}\rfloor} \sum_{k=1}^{+\infty} (k\lfloor\beta_{\{i\}}+1\rfloor + j)^{-\alpha} \\
&\leq \sum_{j=0}^{\lfloor\beta_{\{i\}}\rfloor} \sum_{k=1}^{+\infty} (k\lfloor\beta_{\{i\}}+1\rfloor)^{-\alpha} \\
&\leq \zeta(\alpha)\beta_{\{i\}}^{1-\alpha} \qquad \text{(A.19)}
\end{aligned}$$

and the conclusion for (26) follows. If $\mathfrak{u} = \{i,j\}$, as in (A.19) it is easy to obtain

$$\sum_{\mathbf{k}\in Q_{\{i,j\},\emptyset}} k_i^{-\alpha} k_j^{-\alpha} \leq \frac{\zeta(\alpha)^2}{\beta_{\{i,j\}}^{\alpha-1}}. \qquad \text{(A.20)}$$

And if $\mathfrak{v} = \{i\}$ or $\{j\}$, in view of (A.19) we have

$$\begin{aligned}
\sum_{\mathbf{k}\in Q_{\{i,j\},\mathfrak{v}}} k_i^{-\alpha} k_j^{-\alpha} &= \sum_{k_i=1}^{\lfloor\beta_{\{i,j\}}^{1/2}\rfloor} \sum_{k_j=\beta_{\{i,j\}}/k_i}^{+\infty} k_i^{-\alpha} k_j^{-\alpha} \\
&\leq \sum_{k_i=1}^{\lfloor\beta_{\{i,j\}}^{1/2}\rfloor} \frac{\zeta(\alpha)}{\beta_{\{i,j\}}^{\alpha-1}} k_i^{-1} .
\end{aligned}$$

Then note that the harmonic number $\sum_{k=1}^M k^{-1}$ is bounded by $\log(M)+1$ and deduce

$$\sum_{\mathbf{k}\in Q_{\{i,j\},\mathfrak{v}}} k_i^{-\alpha} k_j^{-\alpha} \leq \frac{\zeta(\alpha)}{\beta_{\{i,j\}}^{\alpha-1}} \big(\log(\beta_{\{i,j\}}^{1/2}) + 1\big) . \qquad \text{(A.21)}$$

Finally, (A.20) and (A.21) gives the conclusion for (27)

$$\sum_{\mathbf{k}\in\mathbb{Z}^*_{\{i,j\}}\setminus K_{\{i,j\}}} \frac{1}{r(\mathbf{k},\alpha,\boldsymbol{\gamma})} \leq \frac{4\gamma_{max}\big[\zeta(\alpha)^2 + 2\zeta(\alpha)\big(\log(\beta_{\{i,j\}}^{1/2}) + 1\big)\big]}{\beta_{\{i,j\}}^{\alpha-1}} .$$

A.6 Proof of Proposition 5

The proof is divided into three parts.

First part. If $f \in \mathcal{H}_\alpha$ then for any $\mathbf{k} \in \mathbb{Z}^d \cap (-\frac{q}{2}, \frac{q}{2}]^d$,

$$|\widehat{\mathrm{c}}_{\mathbf{k}}(f)| = |\mathrm{c}_{\mathbf{k}}(f)| + O(q^{-\alpha/2}) \tag{A.22}$$

and consequently

$$|\widehat{\mathrm{c}}_{\mathbf{k}}(f)|^2 = |\mathrm{c}_{\mathbf{k}}(f)|^2 + O(q^{-\alpha/2}) \ . \tag{A.23}$$

Indeed, Poisson summation formula gives

$$|\widehat{\mathrm{c}}_{\mathbf{k}}(f)| - |\mathrm{c}_{\mathbf{k}}(f)| \leq \sum_{\substack{\mathfrak{u} \subseteq \{1,\ldots,d\} \\ \mathfrak{u} \neq \emptyset}} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{u}}} |\mathrm{c}_{\mathbf{k}+q\mathbf{h}}(f)|$$

and for any non-empty subset $\mathfrak{u} \subseteq \{1, \ldots, d\}$, we have

$$\begin{aligned}
\sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{u}}} |\mathrm{c}_{\mathbf{k}+q\mathbf{h}}(f)| &\leq ||f||_{\mathcal{H}_\alpha} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{u}}} \prod_{i \in \mathfrak{u}} |k_i + qh_i|^{-\alpha/2} \\
&\leq 2^{|\mathfrak{u}|} ||f||_{\mathcal{H}_\alpha} \sum_{h_1=1}^{+\infty} \cdots \sum_{h_{|\mathfrak{u}|}=1}^{+\infty} \prod_{i \in \mathfrak{u}} \left| qh_i - \frac{q}{2} \right|^{-\alpha/2} \\
&\leq q^{-|\mathfrak{u}|\alpha/2} 2^{|\mathfrak{u}|(1+\alpha/2)} ||f||_{\mathcal{H}_\alpha} \sum_{h_1=1}^{+\infty} \cdots \sum_{h_{|\mathfrak{u}|}=1}^{+\infty} \prod_{i \in \mathfrak{u}} |2h_i - 1|^{-\alpha/2} \\
&\leq q^{-|\mathfrak{u}|\alpha/2} 2^{|\mathfrak{u}|(1+\alpha/2)} \zeta\left(\frac{\alpha}{2}\right)^{|\mathfrak{u}|} ||f||_{\mathcal{H}_\alpha} \ .
\end{aligned}$$

Second part. Recall that $\{0, \frac{1}{q}, \ldots \frac{q-1}{q}\}^d$ is denoted by $D(q)$. First we have

$$\begin{aligned}
\mathbb{E}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\Big] &= \frac{1}{|\Pi|} \sum_{\boldsymbol{\pi} \in \Pi} \left(\frac{1}{n} \sum_{i=1}^n f\big((A(\boldsymbol{\pi}))_{i1}, \ldots, (A(\boldsymbol{\pi}))_{id}\big) \right) \\
&= \frac{1}{n} \sum_{i=1}^n \left(\frac{1}{|\Pi|} \sum_{\pi \in \Pi} f\big((A(\boldsymbol{\pi}))_{i1}, \ldots, (A(\boldsymbol{\pi}))_{id}\big) \right) \\
&= \frac{1}{n} \sum_{i=1}^n \left(\frac{1}{q^d} \sum_{\mathbf{x} \in D(q)} f(\mathbf{x}) \right) \\
&= \frac{1}{q^d} \sum_{\mathbf{x} \in D(q)} f(\mathbf{x}) \ .
\end{aligned}$$

Thus, we deduce

$$
\begin{aligned}
\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big)\Big] &= \mathbb{E}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f^2, A(\boldsymbol{\pi})\big) - \widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)^2\Big] \\
&= \mathbb{E}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f^2, A(\boldsymbol{\pi})\big)\Big] - \mathbb{E}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\Big]^2 - \mathrm{Var}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\Big] \\
&= \frac{1}{q^d}\sum_{\mathbf{x}\in D(q)} f(\mathbf{x})^2 - \Bigg(\frac{1}{q^d}\sum_{\mathbf{x}\in D(q)} f(\mathbf{x})\Bigg)^2 - \mathrm{Var}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\Big] \\
&= \mathrm{V}(f) + \widehat{\mathrm{c}}_{\mathbf{0}}(f^2) - \mathrm{c}_{\mathbf{0}}(f^2) + \mathrm{c}_{\mathbf{0}}(f)^2 - \widehat{\mathrm{c}}_{\mathbf{0}}(f)^2 - \mathrm{Var}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\Big]. \qquad \text{(A.24)}
\end{aligned}
$$

We conclude from (A.22) and (A.23)

$$
\mathbb{E}_\mu\Big[\widehat{\mathrm{V}}\big(f, A(\boldsymbol{\pi})\big)\Big] = \mathrm{V}(f) - \mathrm{Var}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\Big] + O\big(q^{-\alpha/2}\big)\ . \qquad \text{(A.25)}
$$

Third part. From Theorem 2, we have

$$
\begin{aligned}
\mathrm{Var}_\mu\Big[\widehat{\mathrm{c}}_{\mathbf{0}}\big(f, A(\boldsymbol{\pi})\big)\Big] &= \frac{1}{n}\sum_{|\mathfrak{u}|\geq 1}\sum_{\mathbf{k}\in\mathbb{Z}^*_{\mathfrak{u}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\big|^2 - \frac{1}{n}\sum_{1\leq|\mathfrak{u}|\leq t}\sum_{\mathbf{k}\in\mathbb{Z}^*_{\mathfrak{u}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\big|^2 \\
&\quad + \frac{1}{n^2}\sum_{|\mathfrak{v}|>t}\Big(-n + \sum_{r=0}^{|\mathfrak{v}|} B(\mathfrak{v}, r)(1-q)^{r-|\mathfrak{v}|}\Big)\sum_{\mathbf{k}\in\mathbb{Z}^*_{\mathfrak{v}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\big|^2\ . \qquad \text{(A.26)}
\end{aligned}
$$

And we now detail the three terms on the right-hand side of (A.26):

i) the first term is

$$
\frac{1}{n}\widehat{\mathrm{V}}(f, D(q)) = \frac{1}{n}\Bigg(\frac{1}{q^d}\sum_{\mathbf{x}\in D(q)} f(\mathbf{x})^2 - \Bigg(\frac{1}{q^d}\sum_{\mathbf{x}\in D(q)} f(\mathbf{x})\Bigg)^2\Bigg)
$$

and is equal to $\frac{1}{n}\big(\mathrm{V}(f) + O(q^{-\alpha/2})\big)$ (see (A.24) and (A.25)).

ii) the second term can be rewritten

$$
-\frac{1}{n}\sum_{1\leq|\mathfrak{u}|\leq t}\Big(\mathrm{V}_{\mathfrak{u}}(f) + \varepsilon_{integ}(\mathfrak{u}) + \varepsilon_{trunc}(\mathfrak{u})\Big)
$$

where, from (A.23), we have

$$
\begin{aligned}
\frac{1}{n}\varepsilon_{integ}(\mathfrak{u}) &= \frac{1}{n}\sum_{\mathbf{k}\in\mathbb{Z}^*_{\mathfrak{u}}(q)}\Big(\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\big|^2 - \big|\mathrm{c}_{\mathbf{k}}(f)\big|^2\Big) \\
&\leq \frac{1}{n}(q-1)^{|\mathfrak{u}|}O(q^{-\alpha/2}) \\
&\leq q^{-t}q^{t}O(q^{-\alpha/2}) \\
&= O(q^{-\alpha/2})
\end{aligned}
$$

and letting for any $\mathfrak{v} \subseteq \mathfrak{u}$,

$$Q'_{\mathfrak{u},\mathfrak{v}} = \{\mathbf{k} \in \mathbb{Z}^*_{\mathfrak{u}},\ \forall i \in \mathfrak{v},\ 1 \leq k_i \leq \frac{q}{2},\ \forall i \in \mathfrak{u} \setminus \mathfrak{v},\ k_i \geq \frac{q}{2}\}$$

we have from (A.19)

$$\begin{aligned}
\frac{1}{n}\varepsilon_{trunc}(\mathfrak{u}) &= \frac{1}{n} \sum_{\mathbf{k} \in \mathbb{Z}^*_{\mathfrak{u}} \setminus \mathbb{Z}^*_{\mathfrak{u}}(q)} \left|c_{\mathbf{k}}(f)\right|^2 \\
&\leq \frac{2^{|\mathfrak{u}|}}{n} ||f||^2_{\mathcal{H}_\alpha} \sum_{\mathfrak{v} \subsetneq \mathfrak{u}} \sum_{\mathbf{k} \in Q'_{\mathfrak{u},\mathfrak{v}}} \prod_{i \in \mathfrak{u}} k_i^{-\alpha} \\
&\leq \frac{2^{|\mathfrak{u}|}}{n} ||f||^2_{\mathcal{H}_\alpha} \sum_{\mathfrak{v} \subsetneq \mathfrak{u}} \Big(\frac{q}{2}\Big)^{|\mathfrak{v}|} \Big(\sum_{k \geq \frac{q}{2}} k^{-\alpha}\Big)^{|\mathfrak{u}|-|\mathfrak{v}|} \\
&\leq \frac{2^{|\mathfrak{u}|}}{n} ||f||^2_{\mathcal{H}_\alpha} \sum_{\mathfrak{v} \subsetneq \mathfrak{u}} \Big(\frac{q}{2}\Big)^{|\mathfrak{v}|} \Big(\zeta(\alpha)\Big(\frac{q}{2}\Big)^{1-\alpha}\Big)^{|\mathfrak{u}|-|\mathfrak{v}|} \\
&\leq \frac{\big(2\zeta(\alpha)\big)^{|\mathfrak{u}|}}{n} ||f||^2_{\mathcal{H}_\alpha} \sum_{\mathfrak{v} \subsetneq \mathfrak{u}} \Big(\frac{q}{2}\Big)^{|\mathfrak{u}|-1} \Big(\frac{q}{2}\Big)^{1-\alpha} \\
&\leq \frac{\big(2\zeta(\alpha)\big)^{|\mathfrak{u}|}}{\lambda q^t} ||f||^2_{\mathcal{H}_\alpha} (2^{|\mathfrak{u}|} - 1) \Big(\frac{q}{2}\Big)^{t-\alpha} \\
&= O(q^{-\alpha})
\end{aligned}$$

iii) as for the third term, note that, since A is defect-free, for all $\mathfrak{v} > t$, $B(\mathfrak{v}, |\mathfrak{v}|) = n$ and for all $i \geq 1$, $B(\mathfrak{v}, t+i) = 0$. Then it comes

$$\begin{aligned}
&\frac{1}{n^2} \sum_{|\mathfrak{v}|>t} \Big(-n + \sum_{r=0}^{|\mathfrak{v}|} B(\mathfrak{v}, r)(1-q)^{r-|\mathfrak{v}|}\Big) \sum_{\mathbf{k} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \left|\widehat{c}_{\mathbf{k}}(f)\right|^2 \\
&\leq \frac{1}{n^2} \sum_{|\mathfrak{v}|>t} \sum_{r=0}^{t} B(\mathfrak{v}, r)(q-1)^{r-|\mathfrak{v}|} \sum_{\mathbf{k} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \Big(\left|c_{\mathbf{k}}(f)\right|^2 + O\big(q^{-\alpha/2}\big)\Big) \\
&\leq \frac{1}{n^2} \sum_{|\mathfrak{v}|>t} \sum_{r=0}^{t} B(\mathfrak{v}, r)(q-1)^{r-|\mathfrak{v}|} \Big(O(1) + O\big(q^{|\mathfrak{v}|-\alpha/2}\big)\Big) \\
&\leq \frac{1}{n^2} \sum_{|\mathfrak{v}|>t} \sum_{r=0}^{t} B(\mathfrak{v}, r)(q-1)^{r} \Big(O(q^{-|\mathfrak{v}|}) + O\big(q^{-\alpha/2}\big)\Big) \\
&\leq O\big(q^{-\min(t+1,\alpha/2)}\big) \frac{1}{n^2} \sum_{|\mathfrak{v}|>t} \sum_{r=0}^{t} B(\mathfrak{v}, r)(q-1)^{r} \\
&\leq O\big(q^{-\min(t+1,\alpha/2)}\big) \qquad \text{(A.27)}
\end{aligned}$$

since for all $r \leq t < |\mathfrak{v}|$, $B(\mathfrak{v}, r) \leq \binom{|\mathfrak{v}|}{r} n^2 q^{-r}$. Indeed, consider

$$B'(\mathfrak{v}, r) = \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbf{1}_{|\{l \in \mathfrak{v},\ A_{il} = A_{jl}\}| \geq r}\ ,$$

we have $B(\mathfrak{v},r) \leq B'(\mathfrak{v},r)$ and it easy to prove that

$$B'(\mathfrak{v},t) = B(\mathfrak{v},t) = \binom{|\mathfrak{v}|}{t} n(nq^{-t}-1)$$

and to deduce that for all $r < t$

$$B'(\mathfrak{v},r) \leq \binom{|\mathfrak{v}|}{r} n(nq^{-r}-1) \ .$$

The conclusion follows.

A.7 Proof of Proposition 6

The proof is divided into three parts.

First part. For any complex-valued random variable Z, define

$$\begin{aligned} \mathrm{Var}[Z] &= \mathbb{E}\Big[\big|Z-\mathbb{E}[Z]\big|^2\Big] \\ &= \mathbb{E}\big[|Z|^2\big] - \big|\mathbb{E}[Z]\big|^2. \end{aligned}$$

Hence, note that $\mathbb{E}_\mu\big[\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big] = \widehat{\mathrm{c}}_{\mathbf{k}}(f)$ and deduce

$$\begin{aligned} \mathbb{E}_\mu\Big[\big|\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big|^2\Big] &= \Big|\mathbb{E}_\mu\big[\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big]\Big|^2 + \mathrm{Var}_\mu\big[\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big] \\ &= \big|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\big|^2 + \mathrm{Var}_\mu\big[\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big] \\ &= \big|\mathrm{c}_{\mathbf{k}}(f)\big|^2 + \mathrm{Var}_\mu\big[\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big] + O\big(q^{-\alpha/2}\big) \end{aligned}$$

where, from Theorem 2, we have

$$\begin{aligned} \mathrm{Var}_\mu\big[\widehat{\mathrm{c}}_{\mathbf{k}}(f, A(\boldsymbol{\pi}))\big] &= \frac{1}{n}\sum_{|\mathfrak{v}|\geq 1}\sum_{\mathbf{h}\in\mathbb{Z}^*_{\mathfrak{v}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\big|^2 - \frac{1}{n}\sum_{1\leq|\mathfrak{v}|\leq t}\sum_{\mathbf{h}\in\mathbb{Z}^*_{\mathfrak{v}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\big|^2 \\ &+ \frac{1}{n^2}\sum_{|\mathfrak{v}|>t}\Big(-n + \sum_{r=0}^{|\mathfrak{v}|} B(\mathfrak{v},r)(1-q)^{r-|\mathfrak{v}|}\Big)\sum_{\mathbf{h}\in\mathbb{Z}^*_{\mathfrak{v}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\big|^2. \end{aligned} \tag{A.28}$$

Denote T_1, T_2 and T_3 the three successive terms on the right-hand side of (A.28). T_3 is given by (A.27) in the proof of Proposition 6, and both the other terms are studied in the next parts.

Second part (details for T_1). Note that for any $\mathfrak{u} \subseteq \{1,\dots,d\}$ and any $\mathbf{k} \in \mathbb{Z}_{\mathfrak{u}}$,

$$\sum_{\mathbf{h}\in\mathbb{Z}_{\mathfrak{u}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\big|^2 = \sum_{\mathbf{h}\in\mathbb{Z}_{\mathfrak{u}}(q)} \big|\widehat{\mathrm{c}}_{\mathbf{h}}(f)\big|^2 \tag{A.29}$$

Indeed, consider

$$\begin{array}{cccc} \Phi_{\mathbf{k}}: & \mathbb{Z}_{\mathfrak{u}}(q) & \longrightarrow & \mathbb{Z}_{\mathfrak{u}}(q) \\ & \mathbf{h} & \longmapsto & \mathbf{h}' \end{array}$$

where for all $i \notin \mathfrak{u}$, $h'_i = 0$, and for $i \in \mathfrak{u}$, h'_i is the remainder in $(-\frac{q}{2}, \frac{q}{2}]$ of the division of $h_i + k_i$ by q. Then, note that

$$\forall \mathbf{h} \in \mathbb{Z}_{\mathfrak{u}}(q), \ \exists \mathbf{l}_0 \in \mathbb{Z}_{\mathfrak{u}}, \ \mathbf{k} + \mathbf{h} = \Phi_{\mathbf{k}}(\mathbf{h}) + q\mathbf{l}_0 \ .$$

Hence, by Poisson summation formula, we have

$$\begin{aligned} \widehat{\mathrm{c}}_{\Phi_{\mathbf{k}}(\mathbf{h})}(f) &= \sum_{\mathbf{l} \in \mathbb{Z}^d} \mathrm{c}_{\Phi_{\mathbf{k}}(\mathbf{h})+q\mathbf{l}}(f) \\ &= \sum_{\mathbf{l} \in \mathbb{Z}^d} \mathrm{c}_{\mathbf{k}+\mathbf{h}+q(\mathbf{l}-\mathbf{l}_0)}(f) \\ &= \widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f) \end{aligned}$$

Finally, noting that $\Phi_{\mathbf{k}}$ is bijective, we conclude to (A.29). Then it comes

$$\begin{aligned} T_1 &= \frac{1}{n} \sum_{|\mathfrak{v}| \geq 1} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \left|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 \\ &= \frac{1}{n} \Bigg(\sum_{\mathbf{h} \in \mathbb{Z}_{\{1,\dots,d\}}(q)} \left|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 - \left|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\right|^2 \Bigg) \\ &= \frac{1}{n} \Bigg(\sum_{\mathbf{h} \in \mathbb{Z}_{\{1,\dots,d\}}(q)} \left|\widehat{\mathrm{c}}_{\mathbf{h}}(f)\right|^2 - \left|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\right|^2 \Bigg) \\ &= \frac{1}{n} \Big(\widehat{\mathrm{V}}(f, D(q)) + \widehat{\mathrm{c}}_{\mathbf{0}}(f)^2 - \left|\widehat{\mathrm{c}}_{\mathbf{k}}(f)\right|^2 \Big) \\ &= \frac{1}{n} \Big(\mathrm{V}(f) + \mathrm{c}_{\mathbf{0}}(f)^2 - \left|\mathrm{c}_{\mathbf{k}}(f)\right|^2 \Big) + O\big(q^{-\alpha/2-t}\big) \end{aligned}$$

Third part (details for T_2). We have

$$\begin{aligned} T_2 &= -\frac{1}{n} \sum_{1 \leq |\mathfrak{v}| \leq t} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \left|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 \\ &= -\frac{1}{n} \sum_{\substack{1 \leq |\mathfrak{v}| \leq t \\ \mathfrak{u} \cap \mathfrak{v} = \emptyset}} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \Big(\left|\mathrm{c}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 + O\big(q^{-\alpha/2}\big) \Big) - \frac{1}{n} \sum_{\substack{1 \leq |\mathfrak{v}| \leq t \\ \mathfrak{u} \cap \mathfrak{v} \neq \emptyset}} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \left|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 \\ &= -\frac{1}{n} \sum_{\substack{1 \leq |\mathfrak{v}| \leq t \\ \mathfrak{u} \cap \mathfrak{v} = \emptyset}} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \left|\mathrm{c}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 - \frac{1}{n} \sum_{\substack{1 \leq |\mathfrak{v}| \leq t \\ \mathfrak{u} \cap \mathfrak{v} \neq \emptyset}} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}}(q)} \left|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 + O(q^{-\alpha/2}) \ . \end{aligned}$$

The first term on the right-hand side is $-R_1(q, t, \lambda, \mathbf{k})/n$ in Proposition 7. The second one, that we denote $R'_2(q, t\lambda, \mathbf{k})$, consists of the sum of $-R_2(q, t, \lambda, \mathbf{k})/n$ and an error term of order $O\big(q^{-\alpha/2}\big)$. Indeed, by an application of the Möbius inversion formula (see e.g. [36]), we have

$$R'_2(q, t\lambda, \mathbf{k}) = -\frac{1}{n} \sum_{\substack{1 \leq |\mathfrak{v}| \leq t \\ \mathfrak{u} \cap \mathfrak{v} \neq \emptyset}} \sum_{\mathfrak{v}' \subseteq \mathfrak{v}} (-1)^{|\mathfrak{v}| - |\mathfrak{v}'|} \sum_{\mathbf{h} \in \mathbb{Z}_{\mathfrak{v}'}(q)} \left|\widehat{\mathrm{c}}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 \ .$$

Now note that (A.29) can be generalized as follows

$$\forall \mathbf{k} \in \mathbb{Z}^d, \quad \sum_{\mathbf{h} \in \mathbb{Z}_{\mathfrak{u}}(q)} \left|\widehat{c}_{\mathbf{k}+\mathbf{h}}(f)\right|^2 = \sum_{\mathbf{h} \in \mathbb{Z}_{\mathfrak{u}}(q)} \left|\widehat{c}_{\mathbf{k}_{\mathfrak{u}}+\mathbf{h}}(f)\right|^2$$

where we recall that $(\mathbf{k}_{\mathfrak{u}})_i = 0$ if $i \in \mathfrak{u}$, and $(\mathbf{k}_{\mathfrak{u}})_i = k_i$ otherwise. Then it comes

$$\begin{aligned}
R_2'(q, t\lambda, \mathbf{k}) &= -\frac{1}{n} \sum_{\substack{1 \le |\mathfrak{v}| \le t \\ \mathfrak{u} \cap \mathfrak{v} \neq \emptyset}} \sum_{\mathfrak{v}' \subseteq \mathfrak{v}} (-1)^{|\mathfrak{v}| - |\mathfrak{v}'|} \sum_{\mathbf{h} \in \mathbb{Z}_{\mathfrak{v}'}(q)} \left|\widehat{c}_{\mathbf{k}_{\mathfrak{v}'}+\mathbf{h}}(f)\right|^2 \\
&= -\frac{1}{n} \sum_{\substack{1 \le |\mathfrak{v}| \le t \\ \mathfrak{u} \cap \mathfrak{v} \neq \emptyset}} \sum_{\mathfrak{v}' \subseteq \mathfrak{v}} (-1)^{|\mathfrak{v}| - |\mathfrak{v}'|} \sum_{\mathfrak{v}'' \subseteq \mathfrak{v}'} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}''}(q)} \left|\widehat{c}_{\mathbf{k}_{\mathfrak{v}'}+\mathbf{h}}(f)\right|^2 \\
&= O\big(q^{-\alpha/2}\big) - \frac{1}{n} \sum_{\substack{1 \le |\mathfrak{v}| \le t \\ \mathfrak{u} \cap \mathfrak{v} \neq \emptyset}} \sum_{\mathfrak{v}' \subseteq \mathfrak{v}} (-1)^{|\mathfrak{v}| - |\mathfrak{v}'|} \sum_{\mathfrak{v}'' \subseteq \mathfrak{v}'} \sum_{\mathbf{h} \in \mathbb{Z}^*_{\mathfrak{v}''}(q)} \left|c_{\mathbf{k}_{\mathfrak{v}'}+\mathbf{h}}(f)\right|^2 .
\end{aligned}$$

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