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A Koksma-Hlawka inequality for simplices

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A Koksma-Hlawka inequality for simplices

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The Koksma-Hlawka inequality gives an estimate of the error in a numerical integration

$$\left| \int_{[0,1]^d} f(x)dx - \frac{1}{N} \sum_{j=1}^{N} f(z_j) \right| \leq \mathcal{D}(z_j) \mathcal{V}(f).$$

Here $\mathcal{D}(z_j)$ is the discrepancy of the finite set of points $\{z_1, \ldots, z_N\}$ in $[0,1)^d$, defined by

$$\mathcal{D}(z_j) = \sup_I \left| |I| - \frac{1}{N} \sum_{j=1}^{N} \chi_I(z_j) \right|,$$

where I is an interval of the form $[0,t_1] \times [0,t_2] \times \ldots \times [0,t_d]$ with $0 < t_k < 1$, and $|I| = t_1 t_2 ... t_d$ is its measure. The term $\mathcal{V}(f)$ is the so-called Hardy-Krause variation, and when f is smooth (say, $\mathcal{C}^d$) this variation takes the form

$$\mathcal{V}(f) = \sum_{\alpha \in \{0,1\}^d, |\alpha| \neq 0} \int_{Q^\alpha} \left| \left(\frac{\partial}{\partial x} \right)^\alpha f(x) \right| dx.$$

The above sum is over all the non vanishing multiindices $\alpha = (\alpha_1, \ldots, \alpha_d)$ which take only the values 0 and 1, $|\alpha|$ is the number of 1's, $(\partial/\partial x)^\alpha = (\partial/\partial x_1)^{\alpha_1} ... (\partial/\partial x_d)^{\alpha_d}$, $Q^\alpha = \left\{ (x_1, \ldots, x_d) \in [0,1]^d : x_j = 1 \text{ if } \alpha_j = 0 \right\}$ is the $|\alpha|$–dimensional face of $[0,1]^d$ parallel to $\alpha_1 e_1, \ldots, \alpha_d e_d$ ($\{e_1, \ldots, e_d\}$ is the canonical basis of $\mathbb{R}^d$) containing the vertex $(1, \ldots, 1)$, and dx is the $|\alpha|$–dimensional Lebesgue surface measure (see [5, 2.5], [6, 1.4], [7, 2.2]). There is an extense literature on this type of estimates, where the contribution to the magnitude of the error given by the irregularity of the point distribution $\{z_1, \ldots, z_N\}$ is isolated from the contribution given by the steepness of the variation of the function f. See e.g. [2], [3], [4], [5], [6], [7], [8]. In [1], one such result has been proven, where the cube $[0,1]^d$ is replaced by a generic bounded Borel subset Ω of $\mathbb{R}^d$. More precisely, let $\{z_1, \ldots, z_N\} \subset [0,1)^d$ be a distribution of N points in the unit cube, and

$$\mathcal{P} = \left\{ z_j + m : j = 1, \ldots, N,\, m \in \mathbb{Z}^d \right\}$$

its periodic extension to the whole Euclidean space $\mathbb{R}^d$. For any $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$ and $t = (t_1, \ldots, t_d) \in (0,1)^d$, let

$$I(x,t) = \cup_{m \in \mathbb{Z}^d} ([0,t_1] \times \ldots \times [0,t_d] + x + m)$$

be the periodic extension of the interval with opposite vertices x and $x+t$. Call $\mathcal{I}$ the collection of all such possible periodic intervals $I(x,t)$. Finally, let $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ be the torus. The main result in [1] is the following.

Theorem 1 *Let f be a smooth $\mathbb{Z}^d$–periodic function on $\mathbb{R}^d$, Ω a bounded Borel subset of $\mathbb{R}^d$, and $\mathcal{P} = \{z_j + m : j = 1, \ldots, N,\ m \in \mathbb{Z}^d\}$ a periodic distribution of points as described above. Then*

$$\left| \int_\Omega f(x)dx - \frac{1}{N} \sum_{z \in \mathcal{P} \cap \Omega} f(z) \right| \leq \mathcal{D}_\mathcal{I}(\Omega, \mathcal{P}) \mathcal{V}_{\mathbb{T}^d}(f),$$

where $\mathcal{D}_\mathcal{I}(\Omega, \mathcal{P})$ is the discrepancy

$$\mathcal{D}_\mathcal{I}(\Omega, \mathcal{P}) = \sup_{I \in \mathcal{I}} \left| |I \cap \Omega| - \frac{1}{N} \sharp (I \cap \Omega \cap \mathcal{P}) \right|,$$

with $|A|$ and $\sharp(A)$ respectively the Lebesgue measure and cardinality of the set A, and $\mathcal{V}_{\mathbb{T}^d}(f)$ is the total variation

$$\mathcal{V}_{\mathbb{T}^d}(f) = \sum_{\alpha \in \{0,1\}^d} 2^{d-|\alpha|} \int_{\mathbb{T}^d} \left| \left(\frac{\partial}{\partial x} \right)^\alpha f(x) \right| dx,$$

where the sum is over all the multiindices α which take only the values 0 and 1, $|\alpha|$ is the number of 1's, and $(\partial/\partial x)^\alpha = (\partial/\partial x_1)^{\alpha_1} \ldots (\partial/\partial x_d)^{\alpha_d}$.

The finite sequence $\{z_1, \ldots, z_N\}$ may present repetitions, but in this case $\sum_{z \in \mathcal{P} \cap \Omega} f(z)$ must be replaced by $\sum_{j=1}^N \sum_{m \in \mathbb{Z}^d} f(z_j + m) \chi_\Omega(z_j + m)$, and similarly $\sharp(I \cap \Omega \cap \mathcal{P})$ by $\sum_{j=1}^N \sum_{m \in \mathbb{Z}^d} \chi_{I \cap \Omega}(z_j + m)$.

When Ω is contained in $[0,1)^d$, the discrepancy $\mathcal{D}_\mathcal{I}(\Omega, \mathcal{P})$ is dominated by $2^d \sup \left| |(B \cap \Omega)| - N^{-1} \sharp (B \cap \Omega \cap \mathcal{P}) \right|$, where the sup is over all the intervals B contained in the unit cube. This reflects the difference between the discrepancy in a torus and the one in a cube, and it is due to the fact that an interval in $\mathbb{T}^d$ can be split into at most 2^d intervals in $[0,1)^d$.

One of the main features of Theorem 1 is the simplicity of its statement, in particular in consideration of the fact that the set Ω is completely arbitrary. On the other hand, observe that the total variation $\mathcal{V}_{\mathbb{T}^d}(f)$ takes into account not only the behaviour of f in Ω, but also the behaviour outside Ω, which is irrelevant in the estimate of

$$\left| \int_\Omega f(x)dx - \frac{1}{N} \sum_{z \in \mathcal{P} \cap \Omega} f(z) \right|.$$

Furthermore, the discrepancy $\mathcal{D}_{\mathcal{I}}(\Omega, \mathcal{P})$ is defined in terms of the family of periodic intervals $\mathcal{I}$, which a priori has no relation with Ω.

The aim of this paper is to show how Theorem 1 can be pushed forward in order to overcome the two above objections, variation of f outside Ω, and introduction of arbitrary "directions" in the discrepancy, and obtain results closer to the original Koksma-Hlawka theorem when Ω is an arbitrary parallelepiped (Theorem 6) or a simplex (Theorem 8) in $\mathbb{R}^d$, f is a smooth function in $\mathbb{R}^d$, not necessarily periodic, and $\mathcal{P}$ is a $\mathbb{Z}^d$–periodic distribution of points.

For the sake of completeness, we sketch here the proof of Theorem 1 (see [1]). In what follows, $\widehat{f}(n) = \int_{\mathbb{T}^d} f(x)e^{-2\pi i n\cdot x}dx$ denotes the Fourier transform and $g * \mu(x) = \int_{\mathbb{T}^d} g(x-y)d\mu(y)$ the convolution, and these operators are applied also to distributions.

Lemma 2 *Let φ be a non vanishing complex sequence on $\mathbb{Z}^d$, and assume that both φ and $1/\varphi$ have tempered growth in $\mathbb{Z}^d$. Also let f be a smooth function on $\mathbb{T}^d$. Define*

$$g(x) = \sum_{n\in\mathbb{Z}^d} \overline{\varphi(n)^{-1}} e^{2\pi i n\cdot x},$$
$$\mathfrak{D}f(x) = \sum_{n\in\mathbb{Z}^d} \varphi(n)\widehat{f}(n)e^{2\pi i n\cdot x}.$$

Finally, let μ be a finite measure on $\mathbb{T}^d$. Then the following identity holds:

$$\int_{\mathbb{T}^d} f(x)\overline{d\mu(x)} = \int_{\mathbb{T}^d} \mathfrak{D}f(x)\,\overline{g*\mu(x)}dx.$$

Lemma 3 *Let the function g on $\mathbb{R}^d$ be the superposition of the characteristic functions of all the periodic intervals $I(0,t)$ with $t\in(0,1]^d$,*

$$g(x) = \int_{(0,1]^d} \chi_{I(0,t)}(x)\,dt.$$

Then the function g has Fourier expansion

$$g(x) = \sum_{n\in\mathbb{Z}^d}\left(\prod_{k=1}^{d}\left(2\delta(n_k)+2\pi i n_k\right)^{-1}\right)e^{2\pi i n\cdot x},$$

where $n=(n_1,...,n_d)$, $\delta(n_k)=1$ if $n_k=0$ and $\delta(n_k)=0$ if $n_k\neq 0$.

Lemma 4 *If f is a smooth function on $\mathbb{T}^d$, then*

$$\mathfrak{D}f(x) = \sum_{n\in\mathbb{Z}^d}\left(\prod_{k=1}^{d}\left(2\delta(n_k)-2\pi i n_k\right)\right)\widehat{f}(n)e^{2\pi i n x}$$
$$= \sum_{\alpha,\beta\in\{0,1\}^d,\ \alpha+\beta=(1,...,1)} (-1)^{|\alpha|}2^{|\beta|}\int_{[0,1]^{|\beta|}}\left(\frac{\partial}{\partial x}\right)^{\alpha} f\left(x+y^{\beta}\right)dy^{\beta}.$$

We are using the notation $(\partial/\partial x)^{\alpha} = (\partial/\partial x_1)^{\alpha_1} \ldots (\partial/\partial x_d)^{\alpha_d}$ *and* $y^{\beta} = \sum_{j=1}^{d} y_j^{\beta_j} e_j$*, where* $\{e_j\}_{j=1}^{d}$ *is the canonical basis of* $\mathbb{R}^d$*, and* $dy^{\beta} = dy_1^{\beta_1} \ldots dy_d^{\beta_d}$*.*

The proofs of the above lemmas are quite straightforward. For the details, see [1].

Proof of Theorem 1. Write $\mu = dx - N^{-1} \sum_{z \in \mathcal{P}} \delta_z$, where δ_z is the point mass centered at z. By Lemma 2 applied to the periodization ν of the measure $\chi_{\Omega}\mu$, and by Hölder inequality, with g and $\mathfrak{D}f$ defined as in Lemma 3 and Lemma 4 respectively,

$$\left| \int_{\Omega} f(x) \overline{d\mu(x)} \right| = \left| \int_{\mathbb{T}^d} f(x) \left(\sum_{n \in \mathbb{Z}^d} \chi_{\Omega}(x+n) \right) \overline{d\mu(x)} \right|$$

$$= \left| \int_{\mathbb{T}^d} f(x) \overline{d\nu(x)} \right| \leq \| \mathfrak{D} f \|_{L^1(\mathbb{T}^d)} \| g * \nu \|_{L^{\infty}(\mathbb{T}^d)} .$$

The estimate for $\| \mathfrak{D} f \|_{L^1(\mathbb{T}^d)}$ follows from Lemma 4,

$$\int_{\mathbb{T}^d} |\mathfrak{D} f(x)| \, dx \leq \sum_{\alpha \in \{0,1\}^d} 2^{d-|\alpha|} \int_{\mathbb{T}^d} \left| \left(\frac{\partial}{\partial x} \right)^{\alpha} f(x) \right| dx.$$

The estimate for $\| g * \nu \|_{L^{\infty}(\mathbb{T}^d)}$ follows from Lemma 3,

$$|g * \nu(x)| = \left| \int_{\mathbb{R}^d} g(x-y) \chi_{\Omega}(y) \, d\mu(y) \right|$$

$$= \left| \int_{\mathbb{R}^d} \int_{(0,1]^d} \chi_{I(0,t)}(x-y) \, dt \chi_{\Omega}(y) \, d\mu(y) \right|$$

$$\leq \int_{(0,1]^d} \left| \int_{\mathbb{R}^d} \chi_{-I(-x,t)}(y) \chi_{\Omega}(y) \, d\mu(y) \right| dt$$

$$\leq \sup_{t \in (0,1]^d} \mu(\Omega \cap (-I(-x,t)))$$

$$\leq \sup_{I \in \mathcal{I}} \left| |I \cap \Omega| - \frac{1}{N} \sharp (I \cap \Omega \cap \mathcal{P}) \right| .$$

■

So far we have followed [1] almost "verbatim". Here we begin some variations on this theme. The next proposition is a first intermediate step in our discussion, and it consists in writing a version of Theorem 1 when Ω is an interval and with $\mathcal{V}_{\mathbb{T}^d}(f)$ replaced by a total variation relative to Ω.

Proposition 5 *Let* f *be a smooth function on* $\mathbb{R}^d$*,* Ω *a compact interval in* $[0,1)^d$*, and* $\mathcal{P} = \{z_j + m : j = 1, \ldots, N, \, m \in \mathbb{Z}^d\}$ *a periodic distribution of points as above. Then*

$$\left| \int_{\Omega} f(x) dx - \frac{1}{N} \sum\nolimits^{*}_{z \in \mathcal{P} \cap \Omega} f(z) \right| \leq \mathcal{D}_{\mathcal{I}}(\Omega, \mathcal{P}) \, \mathcal{V}^{*}_{\Omega}(f),$$

where $\mathcal{V}_{\Omega}^{*}(f)$ *is defined as*

$$\mathcal{V}_{\Omega}^{*}(f)=\sum_{\alpha\in\{0,1\}^{d}}\sum_{\beta\leq\alpha}2^{|\alpha|-|\beta|}\int_{\Omega_{\alpha}}\left|\left(\frac{\partial}{\partial x}\right)^{\beta}f\left(x\right)\right|dx.$$

The symbol $\sum_{z\in\mathcal{P}\cap\Omega}^{*}f\left(z\right)$ *means that if* z *belongs to a* j*–dimensional face of the interval* Ω*, then the term* $f\left(z\right)$ *in the sum must be replaced by* $2^{j-d}f\left(z\right)$*. A multiindex* β *is less than or equal to another multiindex* α *if* $\beta_{j}\leq\alpha_{j}$ *for any* $j=1,\ldots,d$*. Finally* Ω_{α} *is the union of all the* $|\alpha|$*–dimensional faces of* Ω *parallel to the directions* $\alpha_{1}e_{1},\ldots,\alpha_{d}e_{d}$ *(*$\{e_{1},\ldots,e_{d}\}$ *is the canonical basis).*

Proof. Since the problem is translation invariant, we may assume that Ω is contained in $(0,1)^{d}$. Let ϕ be a positive radial smooth function supported on the unit ball and with integral 1, and let $\phi_{\varepsilon}\left(x\right)=\varepsilon^{-d}\phi\left(x/\varepsilon\right)$. Then, for ε small enough, the function $\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}$ (here the convolution is intended in $\mathbb{R}^{d}$) is supported in $(0,1)^{d}$ and can therefore be thought of as the image in the unit cube of a smooth periodic function. Now,

$$\begin{aligned}&\left|\int_{\Omega}f(x)dx-\frac{1}{N}\sum\nolimits_{z\in\mathcal{P}\cap\Omega}^{*}f\left(z\right)\right|\\ \leq\ &\left|\int_{\Omega}\left(f(x)-\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\left(x\right)\right)dx\right|\\ &+\frac{1}{N}\left|\sum_{z\in\mathcal{P}\cap\Omega}\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\left(z\right)-\sum\nolimits_{z\in\mathcal{P}\cap\Omega}^{*}f\left(z\right)\right|\\ &+\left|\int_{\Omega}\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\left(x\right)dx-\frac{1}{N}\sum_{z\in\mathcal{P}\cap\Omega}\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\left(z\right)\right|.\end{aligned}\tag{1}$$

It is well known that $\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\rightarrow f\chi_{\Omega}$ as $\varepsilon\rightarrow0$ in the L^{1} norm. Hence the first term in the above sum goes to zero. As for the second term, observe that if $z\in\mathcal{P}\cap\Omega$ belongs to a j–dimensional face of Ω, then

$$\lim_{\varepsilon\rightarrow0}\int_{\mathbb{R}^{d}}\chi_{\Omega}\left(z-y\right)\phi_{\varepsilon}\left(y\right)dy=2^{j-d}.$$

Similarly,

$$\lim_{\varepsilon\rightarrow0}\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\left(z\right)-2^{j-d}f\left(z\right)=0.$$

Therefore the second term in (1) goes to zero. Finally, we can apply Theorem 1 to the smooth function $\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}$ and obtain

$$\begin{aligned}&\left|\int_{\Omega}\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\left(x\right)dx-\frac{1}{N}\sum_{z\in\mathcal{P}\cap\Omega}\left(f\chi_{\Omega}\right)*\phi_{\varepsilon}\left(z\right)\right|\\ &\leq\mathcal{D}_{\mathcal{I}}\left(\Omega,\mathcal{P}\right)\mathcal{V}_{\mathbb{T}^{d}}(\left(f\chi_{\Omega}\right)*\phi_{\varepsilon})\leq\mathcal{D}_{\mathcal{I}}\left(\Omega,\mathcal{P}\right)\mathcal{V}_{\mathbb{T}^{d}}(f\chi_{\Omega}).\end{aligned}\tag{2}$$

Here $\mathcal{V}_{\mathbb{T}^d}(f\chi_\Omega)$ is defined as before as

$$\mathcal{V}_{\mathbb{T}^d}(f\chi_\Omega)=\sum_{\alpha\in\{0,1\}^d}2^{d-|\alpha|}\int_{\mathbb{T}^d}\left|\left(\frac{\partial}{\partial x}\right)^\alpha(f\chi_\Omega)(x)\right|dx,$$

but now the integral $\int_{\mathbb{T}^d}|(\partial/\partial x)^\alpha(f\chi_\Omega)(x)|\,dx$ must be intended as the total variation of the finite measure $(\partial/\partial x)^\alpha(f\chi_\Omega)$. That this is a measure follows by applying Lebniz rule,

$$\left(\frac{\partial}{\partial x}\right)^\alpha(f\chi_\Omega)(x)=\sum_{\beta+\gamma=\alpha}\left(\frac{\partial}{\partial x}\right)^\beta f(x)\left(\frac{\partial}{\partial x}\right)^\gamma\chi_\Omega(x),$$

and observing that $(\partial/\partial x)^\gamma\chi_\Omega$ is the (signed) surface measure supported on $\Omega_{(1,\ldots,1)-\gamma}$. Thus, the last inequality in (2) follows from the identity

$$\partial/\partial x_j((f\chi_\Omega)*\phi_\varepsilon)=(\partial/\partial x_j(f\chi_\Omega))*\phi_\varepsilon$$

and the inequality

$$\begin{aligned}&\int|((\partial/\partial x)^\alpha(f\chi_\Omega))*\phi_\varepsilon(x)|\,dx\\ &\le\left(\int|(\partial/\partial x)^\alpha(f\chi_\Omega)(x)|\,dx\right)\left(\int|\phi_\varepsilon(x)|\,dx\right).\end{aligned}$$

Finally, again by Leibniz rule,

$$\begin{aligned}\mathcal{V}_{\mathbb{T}^d}(f\chi_\Omega)&=\sum_{\alpha\in\{0,1\}^d}2^{d-|\alpha|}\int_{\mathbb{T}^d}\left|\left(\frac{\partial}{\partial x}\right)^\alpha(f\chi_\Omega)(x)\right|dx\\ &=\sum_{\alpha\in\{0,1\}^d}2^{d-|\alpha|}\int_{\mathbb{R}^d}\left|\sum_{\beta+\gamma=\alpha}\left(\frac{\partial}{\partial x}\right)^\beta f(x)\left(\frac{\partial}{\partial x}\right)^\gamma\chi_\Omega(x)\right|dx\\ &\le\sum_{\alpha\in\{0,1\}^d}2^{d-|\alpha|}\sum_{\beta+\gamma=\alpha}\int_{\Omega_{(1,\ldots,1)-\gamma}}\left|\left(\frac{\partial}{\partial x}\right)^\beta f(x)\right|dx.\end{aligned}$$

Setting $\tilde{\alpha}=(1,\ldots,1)-\alpha+\beta$ gives the desired estimate. ■

A homogeneity argument allows to simplify the total variation $\mathcal{V}^*_\Omega(f)$ in the above proposition. We shall present this argument in the more general context of integration over generic parallelepipeds.

Let Ω be any non degenerate compact parallelepiped in $\mathbb{R}^d$, let W be a $d\times d$ non singular real matrix taking the unit cube $[0,1]^d$ to a translated copy of Ω, and let $w_1,\ldots,w_d\in\mathbb{R}^d$ be its columns. For any multiindex $\alpha\in\{0,1\}^d$, define

$$\left(\frac{\partial}{\partial w}\right)^\alpha f(x)=\left(\frac{\partial}{\partial w_1}\right)^{\alpha_1}\cdots\left(\frac{\partial}{\partial w_d}\right)^{\alpha_d}f(x),$$

where $\partial/\partial w_j=w_j\cdot\nabla$ are the directional derivatives, and define Ω_α as the union of all the $|\alpha|$–dimensional faces of Ω parallel to the directions $\alpha_1w_1,\ldots,\alpha_dw_d$.

Theorem 6 *Let f be a smooth function on $\mathbb{R}^d$, Ω a compact parallelepiped, and $\mathcal{P} = \left\{z_j + m : j = 1, \ldots, N,\ m \in \mathbb{Z}^d\right\}$ a periodic distribution of points. Then*

$$\left|\int_{\Omega} f(x)dx - \frac{1}{N}\sum\nolimits^{*}_{z\in\mathcal{P}\cap\Omega} f(z)\right| \leq \mathcal{D}(\Omega,\mathcal{P})\,\mathcal{V}_{\Omega}(f),$$

where

$$\mathcal{D}(\Omega,\mathcal{P}) = \sup_{I\in\mathcal{I}}\left|\left|W(I)\cap\Omega\right| - \frac{1}{N}\sharp\left(W(I)\cap\Omega\cap\mathcal{P}\right)\right|,$$

is the discrepancy of $\mathcal{P}$ in Ω with respect to (periodic) parallelepipeds parallel to Ω, and

$$\mathcal{V}_{\Omega}(f) = \sum_{\alpha\in\{0,1\}^d} \frac{2^{d-|\alpha|}}{|\Omega_\alpha|}\int_{\Omega_\alpha}\left|\left(\frac{\partial}{\partial w}\right)^{\alpha} f(y)\right| dy$$

is the total variation of f in Ω.

As before, the symbol $\sum^{*}_{z\in\mathcal{P}\cap\Omega} f(z)$ means that if z belongs to a j–dimensional face of the parallelepiped Ω, then the term $f(z)$ in the sum must be replaced by $2^{j-d}f(z)$. The integration over Ω_α is intended with respect to the $|\alpha|$–dimensional Lebesgue surface measure. Observe that, since in Ω_α there are exactly $2^{d-|\alpha|}$ faces, in the definition of total variation the integral is over all possible faces and it is normalized by dividing by the measure of these faces. Also observe that, while in Proposition 5 one integrates over the faces Ω_α all the derivatives of the function f of order $\beta \leq \alpha$, in this theorem the integration is only for $\beta = \alpha$.

It has to be emphasized here that by applying an affine transformation, one can reduce the above problem to the estimate of the error in a numerical integration over the unit square, and then apply the original Koksma-Hlawka inequality. Assuming, for simplicity, that $\Omega = W\left([0,1]^d\right)$, this procedure gives the estimate

$$\begin{aligned} &\left|\int_{\Omega} f(x)dx - \frac{|\Omega|}{n(\mathcal{P},\Omega)}\sum\nolimits_{z\in\mathcal{P}\cap W\left([0,1)^d\right)} f(z)\right| \qquad (3)\\ \leq\ &\sup_{I}\left|\left|W(I)\right| - \frac{|\Omega|}{n(\mathcal{P},\Omega)}\sharp\left(W(I)\cap\mathcal{P}\right)\right| \\ &\times \sum_{\alpha\in\{0,1\}^d,|\alpha|\neq 0}\frac{1}{|\Omega^\alpha|}\int_{\Omega^\alpha}\left|\left(\frac{\partial}{\partial w}\right)^{\alpha} f(x)\right| dx, \end{aligned}$$

where I is an interval of the form $[0,t_1]\times[0,t_2]\times\ldots\times[0,t_d]$ with $0 < t_k < 1$, $n(\mathcal{P},\Omega)$ is the number of points of $\mathcal{P}$ contained in $W\left([0,1)^d\right)$, and Ω^α is the $|\alpha|$–dimensional face of Ω parallel to the directions $\alpha_1 w_1, \ldots, \alpha_d w_d$ containing the vertex $W(1,\ldots,1)$. The disadvantage of (3) with respect to Theorem 6 is in the weight used in the Riemann sums. In Theorem 6 this weight is the inverse of N, which is the exact number of points of $\mathcal{P}$ per unit cube. In (3) the weight is the inverse of $n(\mathcal{P},\Omega)/|\Omega|$, an extrapolation of the number of points per unit cube based on the number of points of $\mathcal{P}$ contained in Ω. As we will see later, in our application to simplices we will need a weight that is independent of the choice of the parallelepiped Ω.

Proof. Without loss of generality, assume that $\Omega = W\left([0,1]^d\right)$. For any integer $m \geq 2$, define the matrix $V = mW$. Observe that $\widetilde{\Omega} := V^{-1}(\Omega) = \left[0, m^{-1}\right]^d$. Also, define the function $\widetilde{f}(x) = f(Vx)$. Thus, the restriction to $\widetilde{\Omega}$ of $\widetilde{f}$ is an "affine image" of the restriction to Ω of the function f. Finally let $\widetilde{\mathcal{P}}$ be the periodic distribution of points obtained by a periodic extension of the set $\left(V^{-1}(\mathcal{P})\right) \cap [0,1)^d$. Call $n\left(\widetilde{\mathcal{P}}\right)$ the cardinality of the set $\left(V^{-1}(\mathcal{P})\right) \cap [0,1)^d$. Then

$$\begin{aligned}
&\left|\int_\Omega f(x)dx - \frac{1}{N}\sum\nolimits^*_{z\in\Omega\cap\mathcal{P}} f(z)\right| \\
= &\left|\int_{\widetilde{\Omega}} f(Vy)\left|\det V\right| dy - \frac{1}{N}\sum\nolimits^*_{z\in\widetilde{\Omega}\cap V^{-1}(\mathcal{P})} f(Vz)\right| \\
= &\left|\det V\right| \left|\int_{\widetilde{\Omega}} \widetilde{f}(y)dy - \frac{1}{N\left|\det V\right|}\sum\nolimits^*_{z\in\widetilde{\Omega}\cap\widetilde{\mathcal{P}}} \widetilde{f}(z)\right|.
\end{aligned}$$

In the last two lines above, the $*$ symbol in the summation signs refers to the faces of the cube $\widetilde{\Omega}$. Observe that we cannot immediately apply Proposition 5 to the last line in the above identities, since $N\left|\det V\right|$ may be different from $n\left(\widetilde{\mathcal{P}}\right)$. Anyhow, Proposition 5 gives

$$\begin{aligned}
&\left|\int_\Omega f(x)dx - \frac{1}{N}\sum\nolimits^*_{z\in\Omega\cap\mathcal{P}} f(z)\right| \\
\leq &\left|\det V\right| \left|\int_{\widetilde{\Omega}} \widetilde{f}(y)dy - \frac{1}{n\left(\widetilde{\mathcal{P}}\right)}\sum\nolimits^*_{z\in\widetilde{\Omega}\cap\widetilde{\mathcal{P}}} \widetilde{f}(z)\right| \\
&+\left|\det V\right| \left|\left(\frac{1}{n\left(\widetilde{\mathcal{P}}\right)} - \frac{1}{N\left|\det V\right|}\right)\sum\nolimits^*_{z\in\widetilde{\Omega}\cap\widetilde{\mathcal{P}}} \widetilde{f}(z)\right| \\
\leq &\left|\det V\right| \mathcal{D}_{\mathcal{I}}\left(\widetilde{\Omega}, \widetilde{\mathcal{P}}\right) \mathcal{V}^*_{\widetilde{\Omega}}\left(\widetilde{f}\right) + \\
&+\left|\det V\right| \left|\left(\frac{1}{n\left(\widetilde{\mathcal{P}}\right)} - \frac{1}{N\left|\det V\right|}\right)\sum\nolimits^*_{z\in\widetilde{\Omega}\cap\widetilde{\mathcal{P}}} \widetilde{f}(z)\right|.
\end{aligned}$$

It turns out that the last term is negligible. Indeed,

$$\begin{aligned}
n\left(\widetilde{\mathcal{P}}\right) &= \sharp\left(\left(V^{-1}\left(\mathcal{P}\right)\right)\cap[0,1)^{d}\right) = \sum_{j=1}^{N}\sum_{k\in\mathbb{Z}^{d}}\chi_{[0,1)^{d}}\left(V^{-1}\left(z_{j}+k\right)\right) \\
&= \sum_{j=1}^{N}\sum_{k\in\mathbb{Z}^{d}}\chi_{V\left([0,1)^{d}\right)}\left(z_{j}+k\right) = \sharp\left(\mathcal{P}\cap V\left([0,1)^{d}\right)\right) \\
&= m^{d}N\left|\Omega\right| + \text{error term.}
\end{aligned}$$

The error term is controlled by N times the number of unit cubes intersecting the boundary of $m\Omega$, thus

$$\text{error term} = \mathcal{O}\left(Nm^{d-1}\right).$$

It follows that

$$\begin{aligned}
&\left|\det V\right|\left|\left(\frac{1}{n\left(\widetilde{\mathcal{P}}\right)}-\frac{1}{N\left|\det V\right|}\right)\sum\nolimits^{*}_{z\in\widetilde{\Omega}\cap\widetilde{\mathcal{P}}}\widetilde{f}\left(z\right)\right| \\
\leq\ & \left|\left(\frac{m^{d}\left|\det W\right|}{Nm^{d}\left|\det W\right|+\mathcal{O}\left(Nm^{d-1}\right)}-\frac{1}{N}\right)\right|\left|\sum\nolimits^{*}_{z\in\mathcal{P}\cap\Omega}f\left(z\right)\right| \\
=\ & \frac{\mathcal{O}\left(m^{-1}\right)}{N}\left|\sum\nolimits^{*}_{z\in\mathcal{P}\cap\Omega}f\left(z\right)\right|
\end{aligned}$$

and this tends to 0 as $m\to+\infty$. Thus we have

$$\left|\int_{\Omega}f(x)dx-\frac{1}{N}\sum\nolimits^{*}_{z\in\mathcal{P}\cap\Omega}f\left(z\right)\right| \leq \lim_{m\to+\infty}\left|\det V\right|\mathcal{D}_{\mathcal{I}}\left(\widetilde{\Omega},\widetilde{\mathcal{P}}\right)\mathcal{V}^{*}_{\widetilde{\Omega}}\left(\widetilde{f}\right).$$

Consider first the discrepancy factor:

$$\begin{aligned}
&\left|\det V\right|\mathcal{D}_{\mathcal{I}}\left(\widetilde{\Omega},\widetilde{\mathcal{P}}\right) \\
&= \left|\det V\right|\sup_{I\subset\mathcal{I}}\left|\left|I\cap\widetilde{\Omega}\right|-\frac{1}{n\left(\widetilde{\mathcal{P}}\right)}\sharp\left(I\cap\widetilde{\Omega}\cap\widetilde{\mathcal{P}}\right)\right| \\
&= \sup_{I\subset\mathcal{I}}\left|\left|V\left(I\right)\cap\Omega\right|-\frac{\left|\det V\right|}{N\left|\det V\right|+\mathcal{O}\left(Nm^{d-1}\right)}\sharp\left(V\left(I\right)\cap\Omega\cap\mathcal{P}\right)\right|.
\end{aligned}$$

Note that, in general, $V\left(\widetilde{\mathcal{P}}\right)$ does not coincide with $\mathcal{P}$, but the above identity holds because $V\left(\widetilde{\Omega}\cap\widetilde{\mathcal{P}}\right)=\Omega\cap\mathcal{P}$. Thus, proceeding as before,

$$\begin{aligned}
&\left|\det V\right|\mathcal{D}_{\mathcal{I}}\left(\widetilde{\Omega},\widetilde{\mathcal{P}}\right) \\
\leq\ & \sup_{I\subset\mathcal{I}}\left|\left|V\left(I\right)\cap\Omega\right|-\frac{1}{N}\sharp\left(V\left(I\right)\cap\Omega\cap\mathcal{P}\right)\right|+\mathcal{O}\left(m^{-1}\right)\sup_{I\subset\mathcal{I}}\frac{1}{N}\sharp\left(V\left(I\right)\cap\Omega\cap\mathcal{P}\right).
\end{aligned}$$

Since

$$\sup_{I\subset\mathcal{I}}\frac{1}{N}\sharp\left(V\left(I\right)\cap\Omega\cap\mathcal{P}\right)\leq C\left|\Omega\right|,$$

then

$$\begin{aligned}\lim_{m\to+\infty}\left|\det V\right|\mathcal{D}_{\mathcal{I}}\left(\widetilde{\Omega},\widetilde{\mathcal{P}}\right) &= \lim_{m\to+\infty}\sup_{I\subset\mathcal{I}}\left|\left|V\left(I\right)\cap\Omega\right|-\frac{1}{N}\sharp\left(V\left(I\right)\cap\Omega\cap\mathcal{P}\right)\right| \\ &= \sup_{I\subset\mathcal{I}}\left|\left|W\left(I\right)\cap\Omega\right|-\frac{1}{N}\sharp\left(W\left(I\right)\cap\Omega\cap\mathcal{P}\right)\right|.\end{aligned}$$

The last identity follows from the fact that, for every positive integer m, the collection of sets $V\left(I\right)\cap\Omega$ coincides with the collection of sets $W\left(I\right)\cap\Omega$. Finally, let us study the variation

$$\begin{aligned}\mathcal{V}^{*}_{\widetilde{\Omega}}\left(\widetilde{f}\right) &= \sum_{\alpha\in\{0,1\}^{d}}\sum_{\beta\leq\alpha}2^{|\alpha|-|\beta|}\int_{\widetilde{\Omega}_{\alpha}}\left|\left(\frac{\partial}{\partial x}\right)^{\beta}\left(f\circ V\right)\left(x\right)\right|dx \\ &= \sum_{\alpha\in\{0,1\}^{d}}\sum_{\beta\leq\alpha}2^{|\alpha|-|\beta|}\frac{\left|\widetilde{\Omega}_{\alpha}\right|}{\left|\Omega_{\alpha}\right|}\int_{\Omega_{\alpha}}\left|\left(\frac{\partial}{\partial x}\right)^{\beta}\left(f\circ V\right)\left(V^{-1}\left(y\right)\right)\right|dy \\ &= \sum_{\alpha\in\{0,1\}^{d}}\sum_{\beta\leq\alpha}2^{|\alpha|-|\beta|}\frac{2^{d-|\alpha|}m^{-|\alpha|}}{\left|\Omega_{\alpha}\right|}\int_{\Omega_{\alpha}}\left|\left(\frac{\partial}{\partial v}\right)^{\beta}f\left(y\right)\right|dy \\ &= \sum_{\alpha\in\{0,1\}^{d}}\sum_{\beta\leq\alpha}2^{|\alpha|-|\beta|}\frac{2^{d-|\alpha|}m^{|\beta|-|\alpha|}}{\left|\Omega_{\alpha}\right|}\int_{\Omega_{\alpha}}\left|\left(\frac{\partial}{\partial w}\right)^{\beta}f\left(y\right)\right|dy.\end{aligned}$$

Finally, when $m\to+\infty$, all the terms in the innermost sum vanish, with the exception of the term with $\beta=\alpha$. Thus,

$$\lim_{m\to+\infty}\mathcal{V}^{*}_{\widetilde{\Omega}}\left(\widetilde{f}\right)=\sum_{\alpha\in\{0,1\}^{d}}\frac{2^{d-|\alpha|}}{\left|\Omega_{\alpha}\right|}\int_{\Omega_{\alpha}}\left|\left(\frac{\partial}{\partial w}\right)^{\alpha}f\left(y\right)\right|dy.$$

■

Our last variation on the Koksma-Hlawka inequality is for simplices. Let now S be a closed simplex in $\mathbb{R}^{d}$, and let $V_0,\ldots,V_d$ be its vertices. For any $k=0,\ldots,d$, let $w^{k}_{1},\ldots,w^{k}_{d}$, be the vectors joining the vertex V_k with the other vertices, in whatever order. Call W_k the matrix with columns $w^{k}_{1},\ldots,w^{k}_{d}$. Let Ω_k be the parallelepiped determined by the vertex V_k and the vectors $w^{k}_{1},\ldots,w^{k}_{d}$. Finally, for every multiindex $\alpha\in\{0,1\}^{d}$, let S^{k}_{α} be the (unique) $|\alpha|$–dimensional face of S parallel to the directions $\alpha_1 w^{k}_{1},\ldots,\alpha_d w^{k}_{d}$. In order to deduce a Koksma-Hlawka inequality for simplices from the Koksma-Hlawka inequality for parallelepipeds, it suffices to decompose the characteristic function of the simplex S into a weighted sum of characteristic functions of the parallelepipeds Ω_k.

Lemma 7 *There exists a constant C_d, depending only on the dimension d, such that for every simplex S there exist smooth functions $\varphi_0, \ldots, \varphi_d$ satisfying the following conditions:*

i) *For every $k = 0, \ldots, d$, we have $\varphi_k(V_k) = 1$, and $\operatorname{supp}(\varphi_k)$ is contained in the open half space determined by the facet of S opposite to V_k.*

ii) $\sum_{k=0}^{d} \varphi_k(x) = 1$ *for every $x \in S$.*

iii) *For all $k = 0, \ldots, d$, and for all multiindices $\alpha \in \{0,1\}^d$,*

$$\sup_{x\in S}\left|\left(\frac{\partial}{\partial w^k}\right)^{\alpha}\varphi_k(x)\right| \leq C_d.$$

Proof. When S is the standard simplex, the lemma follows from a simple partition of unit argument. An affine transformation takes the general simplex onto the standard simplex, without changing the norms in point iii). ■

Theorem 8 *Let f be a smooth function on $\mathbb{R}^d$, S a compact simplex, and $\mathcal{P} = \{z_j + m : j = 1, \ldots, N,\ m \in \mathbb{Z}^d\}$ a periodic distribution of points. Then*

$$\left|\int_S f(x)dx - \frac{1}{N}\sum\nolimits^{*}_{z\in\mathcal{P}\cap S} f(z)\right| \leq \mathcal{D}(S,\mathcal{P})\,\mathcal{V}_S(f),$$

where

$$\mathcal{D}(S,\mathcal{P}) = \max_{k=0,\ldots,d} \mathcal{D}(\Omega_k,\mathcal{P})$$

can be defined as the discrepancy of $\mathcal{P}$ with respect to the $d+1$ parallelepipeds associated with the simplex S, and

$$\mathcal{V}_S(f) = C_d \sum_{k=0}^{d} \sum_{\alpha\in\{0,1\}^d} \sum_{\beta\leq\alpha} \frac{1}{|S^k_\alpha|}\int_{S^k_\alpha}\left|\left(\frac{\partial}{\partial w^k}\right)^{\beta} f(x)\right| dx$$

is the total variation of f in the simplex S.

As before, the symbol $\sum^{*}_{z\in\mathcal{P}\cap\Omega} f(z)$ means that if z belongs to a j–dimensional face of the simplex S, then the term $f(z)$ in the sum must be replaced by $2^{j-d} f(z)$. The integration over S^k_α is intended with respect to the $|\alpha|$–dimensional Lebesgue surface measure. Finally, a multiindex β is less than or equal to another multiindex α if $\beta_j \leq \alpha_j$ for any $j = 1, \ldots, d$.

Proof. Using the partition of unit in the above lemma, we can write

$$\begin{aligned}
&\left|\int_S f(x)\,dx - \frac{1}{N}\sum\nolimits^{*}_{z\in\mathcal{P}\cap S} f(z)\right| \\
=\ &\left|\sum_{k=0}^{d}\left(\int_S f(x)\,\varphi_k(x)\,dx - \frac{1}{N}\sum\nolimits^{*}_{z\in\mathcal{P}\cap S} f(z)\,\varphi_k(z)\right)\right| \\
\leq\ &\sum_{k=0}^{d}\left|\int_{\Omega_k} f(x)\,\varphi_k(x)\,dx - \frac{1}{N}\sum\nolimits^{*}_{z\in\mathcal{P}\cap\Omega_k} f(z)\,\varphi_k(z)\right|.
\end{aligned}$$

By Theorem 6, each term of the above sum is bounded by

$$\sup_{I\in\mathcal{I}}\left||W_k(I)\cap\Omega_k|-\frac{1}{N}\sharp\left(W_k(I)\cap\Omega\cap\mathcal{P}\right)\right|$$
$$\times\sum_{\alpha\in\{0,1\}^d}\frac{2^{d-|\alpha|}}{|\Omega_\alpha^k|}\int_{\Omega_\alpha^k}\left|\left(\frac{\partial}{\partial w^k}\right)^\alpha(f\varphi_k)(y)\right|dy,$$

where Ω_α^k is the union of all the $|\alpha|$–dimensional faces of Ω_k parallel to the directions $\alpha_1 w_1^k,\ldots,\alpha_d w_d^k$. In the above sum, the term corresponding to $\alpha=(0,\ldots,0)$ is just $|f(V_k)|$. When $|\alpha|\neq 0$, by the definition of the functions φ_k, the above integrals over the faces of the parallelepipeds can be replaced by the integrals over the faces of the simplex,

$$\frac{2^{d-|\alpha|}}{|\Omega_\alpha^k|}\int_{\Omega_\alpha^k}\left|\left(\frac{\partial}{\partial w^k}\right)^\alpha(f\varphi_k)(x)\right|dx$$
$$=\frac{1}{|\alpha|\,|S_\alpha^k|}\int_{S_\alpha^k}\left|\left(\frac{\partial}{\partial w^k}\right)^\alpha(f\varphi_k)(x)\right|dx$$

Finally,

$$\left(\frac{\partial}{\partial w^k}\right)^\alpha(f\varphi_k)(x)=\sum_{\beta+\gamma=\alpha}\left(\frac{\partial}{\partial w^k}\right)^\beta f(x)\left(\frac{\partial}{\partial w^k}\right)^\gamma\varphi_k(x).$$

Hence, by the previous lemma,

$$\sum_{\alpha\in\{0,1\}^d}\frac{2^{d-|\alpha|}}{|\Omega_\alpha^k|}\int_{\Omega_\alpha^k}\left|\left(\frac{\partial}{\partial w^k}\right)^\alpha f(y)\right|dy\leq$$
$$\leq\ |f(V_k)|+C_d\sum_{\substack{\alpha\in\{0,1\}^d\\|\alpha|\neq 0}}\sum_{\beta\leq\alpha}\frac{1}{|\alpha|\,|S_\alpha^k|}\int_{S_\alpha^k}\left|\left(\frac{\partial}{\partial w^k}\right)^\beta f(x)\right|dx.$$

■

As an example, let us write explicitly the total variation $\mathcal{V}_S(f)$ in the 2–dimensional case. Let S be a triangle with vertices V_1, V_2 and V_3 . Call l_k the length of the edge S_k opposite to V_k, and w_k the vector joining the two vertices opposite to V_k. Then the variation is

$$\mathcal{V}_S(f) = C_2 |f(V_1)| + C_2 |f(V_2)| + C_2 |f(V_3)|$$
$$+C_2 \frac{2}{l_1} \int_{S_1} \left(|f(x)| + \left| \frac{\partial f}{\partial w_1}(x) \right| \right) dx$$
$$+C_2 \frac{2}{l_2} \int_{S_2} \left(|f(x)| + \left| \frac{\partial f}{\partial w_2}(x) \right| \right) dx$$
$$+C_2 \frac{2}{l_3} \int_{S_3} \left(|f(x)| + \left| \frac{\partial f}{\partial w_3}(x) \right| \right) dx$$
$$+C_2 \frac{1}{|S|} \int_S \left(3|f(x)| + 2\left| \frac{\partial f}{\partial w_1}(x) \right| + 2\left| \frac{\partial f}{\partial w_2}(x) \right| + 2\left| \frac{\partial f}{\partial w_3}(x) \right| + \right.$$
$$\left. + \left| \frac{\partial^2 f}{\partial w_2 \partial w_3}(x) \right| + \left| \frac{\partial^2 f}{\partial w_1 \partial w_3}(x) \right| + \left| \frac{\partial^2 f}{\partial w_1 \partial w_2}(x) \right| \right) dx.$$

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