Weighted L_2 $\mathcal{B}$ Discrepancy and Approximation of Integrals over Reproducing Kernel Hilbert Spaces

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Abstract

We extend the notion of L_2 B discrepancy provided in [E. Novak, H. Woźniakowski, L_2 discrepancy and multivariate integration, in: Analytic number theory. Essays in honour of Klaus Roth. W. W. L. Chen, W. T. Gowers, H. Halberstam, W. M. Schmidt, and R. C. Vaughan (Eds.), Cambridge University Press, Cambridge, 2009, 359 – 388] to the weighted L_2 $\mathcal{B}$ discrepancy. This newly defined notion allows to consider weights, but also volume measures different from the Lebesgue measure and classes of test sets different from measurable subsets of some Euclidean space.

We relate the weighted L_2 $\mathcal{B}$ discrepancy to numerical integration defined over weighted reproducing kernel Hilbert spaces and settle in this way an open problem posed by Novak and Woźniakowski.

1 Introduction

It is known that many notions of geometric L_2 discrepancy are intimately related to multivariate numerical integration over some corresponding reproducing kernel Hilbert spaces, see, e.g., [Zar68, Woź91, Hic98, SW98, NW01a, NW01b, NW09, NW10] and the related literature mentioned therein. In particular, Novak and Woźniakowski introduced in [NW09] (see also [NW10, Chapter 9]) the quite general notion of L_2 B discrepancy. Here B refers to a function that maps elements t from some measurable Euclidean set D to measurable subsets $B(t)$ of $\mathbb{R}^d$. The L_2 B discrepancy of a point set $\{t_1, \ldots, t_n\}$ is then taken with respect to the class of test sets $\mathcal{B} = \{B(t) \,|\, t \in D\}$ and a probability density ρ on D, see Section 4.1 for more details. Novak and Woźniakowski showed that the L_2 B

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discrepancy corresponds to multivariate numerical integration over a Hilbert space with some reproducing kernel K_d related to the class of test sets $\mathcal{B}$ and the probability density ρ.

Their notion of L_2 B discrepancy does not take into account the concept of weights to model the different importance of distinct subsets of coordinates, which is often helpful to overcome the curse of dimensionality. In the context of multivariate numerical integration such weights were probably first studied by Sloan and Woźniakowski in [SW98].

In their new book [NW10] Novak and Woźniakowski posed the open problem to extend the notion of L_2 B discrepancy to include weights and to find relations of the new discrepancy notion to multivariate numerical integration over weighted reproducing kernel Hilbert spaces (cf. [NW10, Open Problem 35]).

In this paper we introduce the even more general definition of weighted L_2 $\mathcal{B}$ discrepancy, which allows not only to consider weights, but also addresses numerical integration with respect to measures that may differ from the Lebesgue measure on domains that are not necessarily measurable subsets of $\mathbb{R}^d$. We prove relations of this discrepancy notion to numerical integration over corresponding weighted reproducing kernel Hilbert spaces and thus settle the open problem posed by Novak and Woźniakowski.

2 Weighted L_2 $\mathcal{B}$ Discrepancy

Let (M, Σ, μ) be a σ-finite measure space. Let $\mathcal{B}$ be a subset of Σ, consisting of sets of finite measure. We assume that there exists a σ-algebra $\Sigma(\mathcal{B})$ on $\mathcal{B}$ and a probability measure ω on $\Sigma(\mathcal{B})$.

Let I be a finite Index set, and for $\nu \in I$ let $(M_\nu, \Sigma_\nu, \mu_\nu)$ be a σ-finite measure space, which is related to the measure space M in the following way: There exists a surjective, measurable map $\Phi_\nu : M \to M_\nu$ such that $\mu_\nu = \mu \circ \Phi_\nu^{-1}$. In particular, we have $\mu_\nu(M_\nu) = \mu(M)$.

Most important for us is the case that Φ_ν is some kind of projection and thus typically a non-injective function. Hence we understand Φ_ν^{-1} not as a function on M_ν, but as a function on the power set of M_ν – it maps each subset A of M_ν to its pre-image $\Phi_\nu^{-1}(A) := \{m \in M \mid \Phi_\nu(m) \in A\}$.

Let $\mathcal{B}_\nu$ be a subset of Σ_ν, consisting of sets of finite measure, endowed with a σ-algebra $\Sigma(\mathcal{B}_\nu)$ and a probability measure ω_ν. We assume for all $\nu \in I$ that the function

$$\chi : \, M_\nu \times B_\nu \to \{0,1\} \, , \, (x_\nu, B_\nu) \mapsto 1_{B_\nu}(x_\nu) \tag{1}$$

is measurable with respect to the product σ-algebra on $M_\nu \times \mathcal{B}_\nu$. It follows that the function

$$B_\nu \mapsto \mu_\nu(B_\nu) = \int_{M_\nu} 1_{B_\nu}(x_\nu) \, \mathrm{d}\mu_\nu(x_\nu)$$

is measurable with respect to $\Sigma(B_\nu)$. Additionally, we require that

$$\int_{\mathcal{B}_\nu} \mu_\nu(B_\nu)^2 \, \mathrm{d}\omega_\nu(B_\nu) < \infty.$$

Now let $\gamma := (\gamma_\nu)_{\nu \in I}$ be a family of non-negative weights. For $\nu \in I$ we define the discrepancy function of a multiset of points $\{t_{1,\nu}, \ldots, t_{n,\nu}\}$ in M_ν for a multiset of real coefficients $\{a_1, \ldots, a_n\}$ and a test set $B_\nu \in \mathcal{B}_\nu$ by

$$\operatorname{disc}(B_\nu, \{t_{j,\nu}\}, \{a_j\}) = \mu_\nu(B_\nu) - \sum_{j=1}^{n} a_j 1_{B_\nu}(t_{j,\nu}), \tag{2}$$

and the weighted L_2 $\mathcal{B}$ discrepancy for a multiset $\{t_1, \ldots, t_n\}$ in M by

$$\operatorname{disc}^{\mathcal{B}}_{2,\gamma}(\{t_j\}, \{a_j\}) = \left(\sum_{\nu \in I} \gamma_\nu \int_{\mathcal{B}_\nu} \operatorname{disc}(B_\nu, \{\Phi_\nu(t_j)\}, \{a_j\})^2 \, \mathrm{d}\omega_\nu(B_\nu) \right)^{1/2}.$$

By using the short hand $t_{j,\nu} := \Phi_\nu(t_j)$ we deduce from (2)

$$\begin{aligned} \operatorname{disc}^{\mathcal{B}}_{2,\gamma}(\{t_j\}, \{a_j\}) = & \Bigg(\sum_{\nu \in I} \gamma_\nu \Bigg[\int_{\mathcal{B}_\nu} \mu_\nu(B_\nu)^2 \, \mathrm{d}\omega_\nu(B_\nu) - 2 \sum_{j=1}^{n} a_j \int_{\mathcal{B}_\nu} \mu_\nu(B_\nu) 1_{B_\nu}(t_{j,\nu}) \, \mathrm{d}\omega_\nu(B_\nu) \\ & + \sum_{i,j=1}^{n} a_i a_j \int_{\mathcal{B}_\nu} 1_{B_\nu}(t_{i,\nu}) 1_{B_\nu}(t_{j,\nu}) \, \mathrm{d}\omega_\nu(B_\nu) \Bigg] \Bigg)^{1/2}. \end{aligned} \tag{3}$$

Let us further define the nth minimal weighted L_2 $\mathcal{B}$ discrepancy $\operatorname{disc}^{\mathcal{B}}_{2,\gamma}(n)$ by

$$\operatorname{disc}^{\mathcal{B}}_{2,\gamma}(n) = \inf\{\operatorname{disc}^{\mathcal{B}}_{2,\gamma}(\{t_j\}, \{a_j\}) \mid t_1, \ldots, t_n \in M, a_1, \ldots, a_n \in \mathbb{R}\}.$$

3 Integration on Weighted Reproducing Kernel Hilbert Spaces

Let $(\widetilde{K}_\nu)_{\nu \in I}$ be a family of reproducing kernels $\widetilde{K}_\nu : M_\nu \times M_\nu \to \mathbb{R}$. Then for each $\nu \in I$ the function K_ν, defined by

$$K_\nu(x, y) = \widetilde{K}_\nu(\Phi_\nu(x), \Phi_\nu(y)) \quad \text{for all } x, y \in M,$$

is a reproducing kernel on $M \times M$ (since K_ν inherits from $\widetilde{K}_\nu$ the sufficient properties of symmetry and of positive semi-definiteness). Let us define the weighted reproducing kernel K_γ on $M \times M$ by

$$K_\gamma(x, y) = \sum_{\nu \in I} \gamma_\nu K_\nu(x, y) \quad \text{for all } x, y \in M, \tag{4}$$

and let $H(K_\gamma)$ be the corresponding reproducing kernel Hilbert space of functions defined on M. We assume that $H(K_\gamma)$ consists of integrable functions with respect to μ and that the integral

$$\mathcal{I}(f) = \int_M f(x) \, \mathrm{d}\mu(x)$$

is a bounded linear functional on $H(K_\gamma)$, i.e, that the function

$$h_\gamma := \int_M K_\gamma(x,\cdot)\,\mathrm{d}\mu(x) \in H(K_\gamma).$$

Note that

$$I(f) = \langle f, h_\gamma\rangle_{H(K_\gamma)} \quad \text{for all } f \in H(K_\gamma).$$

Let Q_n be a linear algorithm given by

$$Q_n(f) = \sum_{j=1}^n a_j f(t_j)$$

with $\{t_1,\dots,t_n\} \in M$ and real coefficients $\{a_1,\dots,a_n\}$. Then

$$\mathcal{I}(f) - Q_n(f) = \langle f, h_{\gamma,n}\rangle_{H(K_\gamma)} \quad \text{for all } f \in H(K_\gamma),$$

where

$$h_{\gamma,n} := h_\gamma - \sum_{j=1}^n a_j K_\gamma(t_j,\cdot).$$

If we want to approximate the functional $\mathcal{I}$ by the linear algorithm Q_n, then the worst case error of the approximation taken over the norm unit ball of $H(K_\gamma)$ is given by

$$e^{\mathrm{wor}}(\mathcal{I}, Q_n, H(K_\gamma)) = \sup_{\|f\|_{H(K_\gamma)}\le 1} |\mathcal{I}(f) - Q_n(f)| = \|h_{\gamma,n}\|_{H(K_\gamma)}. \tag{5}$$

This leads to

$$\begin{aligned}
&e^{\mathrm{wor}}(\mathcal{I}, Q_n, H(K_\gamma))^2 \\
=&\|h_\gamma\|^2_{H(K_\gamma)} - 2\sum_{j=1}^n a_j \langle h_\gamma, K_\gamma(t_j,\cdot)\rangle_{H(K_\gamma)} + \sum_{i,j=1}^n a_i a_j \langle K_\gamma(t_i,\cdot), K_\gamma(t_j,\cdot)\rangle_{H(K_\gamma)} \\
=&\int_M\int_M K_\gamma(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y) - 2\sum_{j=1}^n a_j \int_M K_\gamma(t_j,x)\,\mathrm{d}\mu(x) + \sum_{i,j=1}^n a_i a_j K_\gamma(t_i,t_j) \\
=&\sum_{\nu\in I}\gamma_\nu \left[\int_M\int_M K_\nu(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y) - 2\sum_{j=1}^n a_j \int_M K_\nu(t_j,x)\,\mathrm{d}\mu(x) + \sum_{i,j=1}^n a_i a_j K_\nu(t_i,t_j)\right].
\end{aligned}$$

Let us also define the nth minimal worst case error $e^{\mathrm{wor}}(n, H(K_\gamma))$ by

$$e^{\mathrm{wor}}(n, H(K_\gamma)) = \inf\{e^{\mathrm{wor}}(\mathcal{I}, Q_n, H(K_\gamma)) \,|\, Q_n \text{ with arbitrary } t_j \text{ and } a_j\}.$$

If we want the identity

$$e^{\mathrm{wor}}(\mathcal{I}, Q_n, H(K_\gamma)) = \mathrm{disc}^{\mathcal{B}}_{2,\gamma}(\{t_j\},\{a_j\}) \tag{6}$$

to hold no matter how we choose the finite sequences $\{t_j\}$, $\{a_j\}$, and $\gamma = \{\gamma_\nu\}$, then we necessarily have to require that

$$K_\nu(x,y) = \int_{\mathcal{B}_\nu} 1_{B_\nu}(\Phi_\nu(x)) 1_{B_\nu}(\Phi_\nu(y)) \,\mathrm{d}\omega_\nu(B_\nu) \quad \text{for all } x, y \in M \text{ and all } \nu \in I. \tag{7}$$

Condition (7) is not only necessary, but also sufficient for (6) to hold independently of the choice of the finite sequences $\{t_j\}$, $\{a_j\}$, and $\gamma = \{\gamma_\nu\}$, since, due to our assumptions $\mu_\nu = \mu \circ \Phi_\nu^{-1}$ and the measurability of χ defined in (1), and to the theorem of Fubini and Tonelli,

$$\begin{aligned}
\int_M \int_M K_\nu(x,y) \,\mathrm{d}\mu(x) \,\mathrm{d}\mu(y) &= \int_M \int_M \int_{\mathcal{B}_\nu} 1_{B_\nu}(\Phi_\nu(x)) 1_{B_\nu}(\Phi_\nu(y)) \,\mathrm{d}\omega_\nu(B_\nu) \,\mathrm{d}\mu(x) \,\mathrm{d}\mu(y) \\
&= \int_{\mathcal{B}_\nu} \left(\int_M 1_{B_\nu}(\Phi_\nu(x)) \,\mathrm{d}\mu(x) \right)^2 \mathrm{d}\omega_\nu(B_\nu) \\
&= \int_{\mathcal{B}_\nu} \left(\int_{M_\nu} 1_{B_\nu}(\xi_\nu) \,\mathrm{d}\mu_\nu(\xi_\nu) \right)^2 \mathrm{d}\omega_\nu(B_\nu) \\
&= \int_{\mathcal{B}_\nu} \mu_\nu(B_\nu)^2 \,\mathrm{d}\omega_\nu(B_\nu).
\end{aligned}$$

Furthermore,

$$\begin{aligned}
\int_M K_\nu(t_j, x) \,\mathrm{d}\mu(x) &= \int_{\mathcal{B}_\nu} 1_{B_\nu}(\Phi_\nu(t_j)) \left(\int_M 1_{B_\nu}(\Phi_\nu(x)) \,\mathrm{d}\mu(x) \right) \mathrm{d}\omega_\nu(B_\nu) \\
&= \int_{\mathcal{B}_\nu} 1_{B_\nu}(\Phi_\nu(t_j)) \mu_\nu(B_\nu) \,\mathrm{d}\omega_\nu(B_\nu).
\end{aligned}$$

Hence identity (6) follows from identity (3).

Let us still assume that condition (7) holds. If (M, Σ, μ) is a finite measure space, i.e., if $\mu(M) < \infty$, then we can prove an upper bound on $e^{\mathrm{wor}}(n, H(K_\gamma))$ by averaging over all properly normalized quasi-Monte Carlo algorithms. More precisely, we proceed similarly as in [NW09] and consider algorithms of the form

$$Q_n(f) = \frac{\mu(M)}{n} \sum_{j=1}^n f(t_j) \tag{8}$$

and average the square of the worst-case error

$$f(t_1, \dots, t_n) := e^{\mathrm{wor}}(\mathcal{I}, Q_n, H(K_\gamma))^2$$

over all n-point multisets $\{t_1, \dots, t_n\}$ in M:

$$\begin{aligned}
&\frac{1}{\mu(M)^n} \int_{M^n} f(t_1, \dots, t_n) \, \mathrm{d}\mu(t_1) \dots \, \mathrm{d}\mu(t_n) \\
=&\frac{1}{n} \sum_{\nu \in I} \gamma_\nu \left[\mu(M) \int_M K_\nu(x,x) \, \mathrm{d}\mu(x) - \int_M \int_M K_\nu(x,y) \, \mathrm{d}\mu(x) \, \mathrm{d}\mu(y) \right] \\
=&\frac{1}{n} \sum_{\nu \in I} \gamma_\nu \left[\mu_\nu(M_\nu) \int_{\mathcal{B}_\nu} \mu_\nu(B_\nu) \, \mathrm{d}\omega_\nu(B_\nu) - \int_{\mathcal{B}_\nu} \mu_\nu(B_\nu)^2 \, \mathrm{d}\omega_\nu(B_\nu) \right] \\
\le&\frac{1}{n} \sum_{\nu \in I} \gamma_\nu \mu_\nu(M_\nu)^2 = \frac{\mu(M)^2}{n} \sum_{\nu \in I} \gamma_\nu .
\end{aligned}$$

From this it follows directly that at least for one normalized quasi-Monte Carlo algorithm Q_n of the form (8) we have the estimate

$$e^{\mathrm{wor}}(\mathcal{I}, Q_n, H(K_\gamma)) \le \frac{\mu(M) \sqrt{\sum_{\nu \in I} \gamma_\nu}}{\sqrt{n}} .$$

Altogether we have proved the following theorem.

Theorem 3.1. *Under the assumptions made above, we have for a weighted reproducing kernel K_γ defined by equation (4), which satisfies additionally condition (7), that the identity*

$$e^{\mathrm{wor}}(\mathcal{I}, Q_n, H(K_\gamma)) = \mathrm{disc}^{\mathcal{B}}_{2,\gamma}(\{t_j\}, \{a_j\})$$

holds for all linear algorithms $Q_n(f) = \sum_{j=1}^n a_j f(t_j)$. Consequently, we have

$$e^{\mathrm{wor}}(n, H(K_\gamma)) = \mathrm{disc}^{\mathcal{B}}_{2,\gamma}(n).$$

If additionally $\mu(M) < \infty$ holds, then

$$e^{\mathrm{wor}}(n, H(K_\gamma)) \le \frac{\mu(M) \sqrt{\sum_{\nu \in I} \gamma_\nu}}{\sqrt{n}} .$$

4 Special Cases

Here we want to discuss some special cases of the quite general notion of weighted L_2 $\mathcal{B}$ discrepancy from Section 2.

4.1 L_2 B Discrepancy

We start with the L_2 B discrepancy as defined in [NW09], see also [NW10]. This discrepancy fits in our more general definition if we make the following choices: Let M be a measurable subset of $\mathbb{R}^d$, Σ be the Borel σ-algebra and μ be the d-dimensional Lebesgue measure restricted to M. Let $\mathcal{B}$ be a class of measurable subsets of $\mathbb{R}^d$ with $\cup_{B \in \mathcal{B}} B = M$.

For a given function $\tau : \mathbb{N} \to \mathbb{N}$ let $D \subseteq \mathbb{R}^{\tau(d)}$ be Borel measurable and $\rho : D \to [0, \infty)$ a probability density. Let the σ-algebra $\sum(\mathcal{B})$ on $\mathcal{B}$ be induced by a parametrization $T : D \to \mathcal{B}$, $t \mapsto B(t)$ such that the mapping $(t, x) \mapsto 1_{B(t)}(x)$ is measurable on $D \times M$ with respect to the product σ-algebra. (The last important measurability condition was indeed forgotten in [NW09], but is added in the more recent and more comprehensive exposition [NW10, Chapter 9].)

Let the probability measure ω on $\mathcal{B}$ be induced by the probability measure $\rho(t)\,\mathrm{d}t$, where $\mathrm{d}t$ is the $\tau(d)$-dimensional Lebesgue measure. Furthermore, let $I = \{1\}$, $\gamma_1 = 1$, and let $\Phi_1 : M \to M$ be the identity mapping.

For these special choices the weighted L_2 $\mathcal{B}$ discrepancy is nothing but the L_2 B discrepancy as defined in [NW09]. In this situation our Theorem 3.1 was already proved in [NW09].

4.2 Weighted L_2 Star Discrepancy

To get from our definition of weighted L_2 $\mathcal{B}$ discrepancy the special case of the weighted L_2 star discrepancy (which is sometimes also called weighted L_2 discrepancy anchored at 0), we just have to make the following choices:

Let $M = [0, 1]^d$, Σ the Borel σ-algebra on $[0, 1]^d$, μ the restriction of the Lebesgue measure to $[0, 1]^d$, and $\mathcal{B} = \{[0, x) \,|\, x \in [0, 1]^d\}$, where $[0, x) = [0, x_1) \times \cdots \times [0, x_d)$ for a vector $x = (x_1, \ldots, x_d)$. As a measure space we identify $\mathcal{B}$ via the mapping $\iota : [0, 1]^d \to \mathcal{B}$, $x \mapsto [0, x)$ with the measure space (M, Σ, μ). (Note that ι is not a bijection, since $\iota(x) = \emptyset$ for all $x \in \{y \in [0, 1]^d \,|\, \exists i : y_i = 0\}$; but this is irrelevant for our purpose, since the latter set has Lebesgue measure zero.)

Let $I = \{u \,|\, u \subseteq [d]\}$, where $[d] := \{1, \ldots, d\}$. Let $M_u = [0, 1]^{|u|}$, where $|u|$ denotes the cardinality of the set u, and let

$$\Phi_u : [0, 1]^d \to [0, 1]^{|u|}\,,\; x = (x_i)_{i=1}^d \mapsto (x_\nu)_{\nu \in u}.$$

Then $\mu_u = \mu \circ \Phi_u^{-1}$ is nothing but the restriction of the $|u|$-dimensional Lebesgue measure to $[0, 1]^{|u|}$. Furthermore, let $\mathcal{B}_u = \{[0, \xi_u) \,|\, \xi_u \in [0, 1]^{|u|}\}$ and identify $\mathcal{B}_u$ as a measure space with (M_u, Σ_u, μ_u).

Condition (7) reads now as follows:

$$\begin{aligned}
\int_{\mathcal{B}_u} 1_{B_u}(\Phi_u(x)) 1_{B_u}(\Phi_u(y))\,\mathrm{d}\omega_u(B_u) &= \int_{[0,1]^{|u|}} 1_{[0,\xi_u)}(\Phi_u(x)) 1_{[0,\xi_u)}(\Phi_u(y))\,\mathrm{d}\xi_u \\
&= \prod_{\nu \in u} \int_0^1 1_{[0,\xi)}(x_\nu) 1_{[0,\xi)}(y_\nu)\,\mathrm{d}\xi \\
&= \prod_{\nu \in u} (1 - \max\{x_\nu, y_\nu\}).
\end{aligned}$$

This leads us to the weighted reproducing kernel

$$K_\gamma(x, y) = \sum_{u \subseteq [d]} \gamma_u K_u(x, y),$$

where, by using the short hand $\widetilde{K}(\xi,\eta) = 1 - \max\{\xi,\eta\}$,

$$K_u(x,y) = \prod_{\nu\in u} \widetilde{K}(x_\nu, y_\nu).$$

The resulting Hilbert space is the weighted Sobolev space with mixed derivatives of order 1 anchored at 1, and is, e.g., discussed in detail in [NW09, NW10]. In this situation Theorem 3.1 was proved in [SW98] for so-called product weights. For general weights the result can be found in [NW09].

Notice that, due to the product structure of the classes of test sets

$$\mathcal{B}_u = \left\{ \prod_{\nu\in u} [0, x_\nu) \,\middle|\, \forall \nu \in u :\, x_\nu \in [0,1] \right\},$$

the measures $\omega_u = \mathrm{d}\xi_u = \otimes_{\nu\in u}\mathrm{d}\xi$, and of the kernels

$$K_u(x,y) = \prod_{\nu\in u} \widetilde{K}(x_\nu, y_\nu),$$

condition (7) is equivalent to

$$\widetilde{K}(r,s) = \int_0^1 1_{[0,t)}(r) 1_{[0,t)}(s)\,\mathrm{d}s \quad \forall r,s \in [0,1]. \tag{9}$$

This observation will be generalized in the extended final version of this draft paper; there also more examples, like the so-called G-discrepancy and H-discrepancy which have applications in quasi-Monte Carlo importance sampling and for which μ may differ from the Lebesgue measure, will be discussed. Furthermore, we will study infinite dimensional integration—this can formally be done by considering also infinite sets of indices I, but nevertheless one has to modify the definition of the numerical integration problem given in this draft paper appropriately.

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