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A link between the Hoeffding–Sobol and Möbius decompositions

Cécile Mercadier^{a,*}, Olivier Roustant^b, Christian Genest^c

^a*Univ Lyon, Université Claude Bernard Lyon 1, CNRS UMR 5208, Institut Camille Jordan F-69622 Villeurbanne, France.*

^b*Institut de Mathématiques de Toulouse, Université de Toulouse, INSA, Toulouse, 31077 cedex 4, France.*

^c*Department of Mathematics and Statistics, McGill University, 805, rue Sherbrooke ouest, Montréal, Québec, Canada H3A 0B9.*

Abstract

The Hoeffding–Sobol and Möbius decompositions are two different ways of writing a multivariate function as a sum of components having successively fewer variables. The Hoeffding–Sobol decomposition is used extensively in global sensitivity analysis, while the Möbius decomposition has found applications in the theory of tests of independence. It is shown here that both of these formulae derive from a result of Kuo, Sloan, Wasilkowski, and Woźniakowski (*Math. Comp.*, 79 (2010), no. 270, pp. 953–966) concerning the representation of multivariate functions through projections. The relative merits of the two formulae are also highlighted.

Keywords: Hoeffding–Sobol decomposition, Möbius decomposition, Functional representation, Annihilating property

2010 MSC: 41A63, 46N30

1. Introduction

As its title announces, this note aims to elucidate the connection between the Hoeffding–Sobol and Möbius decompositions. Developed in different contexts, both of these formulae make it possible to express a real-valued function f of $d \geq 2$ variables acting on a domain $D \subseteq \mathbb{R}^d$ into a sum running over all subsets u of $\{1, \dots, d\}$. Namely

$$f = \sum_{u \subseteq \{1, \dots, d\}} f_u, \quad (1)$$

where f_u is a function of the variables with indices in u alone, with the convention that the map f_\emptyset is a constant. Thus, the terms in the sum (1) become simpler and simpler as the size $|u|$ of the set u decreases from d to zero.

The Hoeffding–Sobol decomposition goes back to the seminal work of Hoeffding on the theory of U -statistics [1], and by analogy with analysis of variance, Sobol [2] used it to derive sensitivity indices from the elements of the decomposition. This decomposition, whose definition will be recalled later in this note, has found many applications in statistics, notably in global sensitivity analysis; see, e.g., [3, 4, 5, 6, 7, 8, 9]. In particular, the Hoeffding–Sobol decomposition has been used extensively to compare the performance of Monte Carlo versus quasi-Monte Carlo integration in high-dimensional integration problems, given that the notion of effective dimension reduces the dimension of the domain of integration; see, e.g., [10, 11, 12]. More recently, the Hoeffding–Sobol decomposition

*Corresponding author

Email address: mercadier@math.univ-lyon1.fr (Cécile Mercadier)

11 has also been used to define and study the tail dependograph, a graphical tool which captures the structure of
 12 asymptotic dependence within a multivariate random phenomena; see [13, 14].

13 By comparison, the Möbius decomposition is relatively unknown. It was originally suggested by Deheuvels [15]
 14 as a way to construct rank-based tests of independence among the components of a continuous random vector.
 15 More specifically, an application of the Möbius combinatorial formula leads to a representation of an empirical
 16 copula, and hence also of the empirical copula process, into a finite number of components which, under the null
 17 hypothesis of independence, are asymptotically independent. Cramér–von Mises statistics derived from the sub-
 18 processes prove to be very powerful, both asymptotically and in finite samples [16, 17, 18]. This approach has since
 19 been extended to the problem of testing for independence between random vectors [19, 20], and more recently to
 20 testing for dependence between arbitrary random variables [21].

21 Because the Hoeffding–Sobol and Möbius formulae were developed in different contexts, the connection between
 22 them has never been spelled out. It is shown here that they are linked through a general representation for
 23 multivariate functions due to [22] which is described in Section 2. The way in which this general expression can be
 24 used to obtain the two decomposition formulae is then detailed in Section 3. These calculations suggest a slight
 25 extension of the result by [22] which is stated and proved in Section 4. This is followed in Section 5 by a short
 26 discussion of the comparative advantages of the Hoeffding–Sobol and Möbius decompositions.

27 2. A general decomposition formula

28 Let \mathcal{F} be the linear space of real-valued functions acting on a domain $D \subseteq \mathbb{R}^d$ and for each $i \in \{1, \dots, d\}$, let
 29 $P_i : \mathcal{F} \rightarrow \mathcal{F}$ be a projection, i.e., a map whose composition with itself, denoted $P_i P_i$, returns P_i . Further assume
 30 that these projections are commuting, i.e., for any distinct $i, j \in \{1, \dots, d\}$, $P_i P_j = P_j P_i$, and let I_D denote the
 31 identity operator on \mathcal{F} .

Kuo et al. [22] gave conditions on the projections P_1, \dots, P_d which ensure both the existence and uniqueness of
 the decomposition (1) based on terms defined, for any function $f \in \mathcal{F}$ and arbitrary subset $u \subseteq \{1, \dots, d\}$, by

$$f_u = \left(\prod_{i \in u} (I_D - P_i) \prod_{i \notin u} P_i \right) (f). \quad (2)$$

32 Their result holds provided that each projection eliminates the dependence on a specific input variable to which
 33 the function is applied. To describe this finding, introduce, for each set $u \subseteq \{1, \dots, d\}$, the class \mathcal{F}_u of functions
 34 $f \in \mathcal{F}$ such that $f(x_1, \dots, x_d) = f(y_1, \dots, y_d)$ when $x_j = y_j$ for all $j \in u$. Elements of \mathcal{F}_u are then maps $f \in \mathcal{F}$ such
 35 that $f(\mathbf{x})$ depends only on the coordinates of \mathbf{x} whose index is in u , and hence \mathcal{F}_\emptyset is the set of constant functions.
 36 To simplify notation, write $\mathcal{F}_{-i} = \mathcal{F}_{\{1, \dots, d\} \setminus \{i\}}$ for all $i \in \{1, \dots, d\}$.

37 The key assumption in Theorem 2.1 of [22], formally stated below, means that for any $i \in \{1, \dots, d\}$ and $f \in \mathcal{F}$,
 38 the value of $P_i(f)$ at \mathbf{x} does not depend on the i th coordinate of \mathbf{x} and that if f does not depend at all on this
 39 coordinate, the projection P_i leaves the function unchanged.

Assumption 1. For all $i \in \{1, \dots, d\}$ and $f \in \mathcal{F}$,

$$P_i(f) \in \mathcal{F}_{-i}, \quad (3)$$

$$f \in \mathcal{F}_{-i} \Rightarrow P_i(f) = f. \quad (4)$$

40 In what follows, for any set $u \subseteq \{1, \dots, d\}$ and vector $\mathbf{x} \in D$, \mathbf{x}_u stands for a vector whose length is the
 41 cardinality $|u|$ of u and whose components are those of \mathbf{x} whose indices are in u .

42 **Proposition 1.** *Let \mathcal{F} be a linear space of real-valued functions acting on a domain $D \subseteq \mathbb{R}^d$ and let P_1, \dots, P_d be
 43 commuting projections on \mathcal{F} that satisfy Assumption 1. Then, any function $f \in \mathcal{F}$ can be expressed in the form (1),
 44 where the map f_u defined in (2) is such that for any vector $\mathbf{x} \in D$, $f_u(\mathbf{x})$ only depends on \mathbf{x}_u .*

45 The second part of Theorem 2.1 of [22] is stated separately below for added clarity. Condition (5) therein is
 46 termed the annihilating property by these authors.

Proposition 2. *Under the same conditions as in Proposition 1, suppose that every $f \in \mathcal{F}$ can be written in the
 form (1) and that $f_u \in \mathcal{F}_u$ for every set $u \subseteq \{1, \dots, d\}$. Further assume that, for all $i \in \{1, \dots, d\}$,*

$$P_i(f_u) = \begin{cases} 0 & \text{if } i \in u, \\ f_u & \text{if } i \notin u. \end{cases} \quad (5)$$

Then, the term f_u given in (2) satisfies the recursive relation

$$f_u = P_{\{1, \dots, d\} \setminus u}(f) - \sum_{v \subsetneq u} f_v, \quad (6)$$

where for any set $u \subseteq \{1, \dots, d\}$, $P_u = \prod_{i \in u} P_i$. Furthermore, one has

$$f_u = \sum_{v \subseteq u} (-1)^{|u \setminus v|} P_{\{1, \dots, d\} \setminus v}(f). \quad (7)$$

47 3. Special cases of Proposition 1

48 It is shown below that the Hoeffding–Sobol and Möbius decompositions are special cases of Proposition 1.

Considering first the Hoeffding–Sobol decomposition, let $\mathcal{F} = L^2(D)$ be the collection of square integrable
 functions on $D = [0, 1]^d$. For each $i \in \{1, \dots, d\}$, let the projection P_i be defined through integration with respect
 to the i th variable. That is, for every function $f \in \mathcal{F}$ and vector $\mathbf{x} = (x_1, \dots, x_d) \in [0, 1]^d$, set

$$P_i(f)(\mathbf{x}) = \int_0^1 f(x_1, \dots, x_{i-1}, z, x_{i+1}, \dots, x_d) dz.$$

Alternatively, the projection P_i could be defined as an expectation with respect to the i th component of a vector
 $\mathbf{Z} = (Z_1, \dots, Z_d)$ of mutually independent random variables uniformly distributed on the interval $[0, 1]$. Indeed, for
 every function $f \in \mathcal{F}$ and vector $\mathbf{x} = (x_1, \dots, x_d) \in [0, 1]^d$,

$$P_i(f)(\mathbf{x}) = \mathbb{E}[f(x_1, \dots, x_{i-1}, Z_i, x_{i+1}, \dots, x_d)].$$

It is clear that the maps P_1, \dots, P_d so defined are commuting projections that satisfy (1). The well-known
 Hoeffding–Sobol decomposition then results upon injecting these projections into formula (2). Indeed, given that
 the terms in expression (2) are mutually orthogonal in the L^2 -sense, it is easily checked that

$$\text{var}(f(\mathbf{Z})) = \sum_{u \subseteq \{1, \dots, d\}} \text{var}(f_u(\mathbf{Z})),$$

so that the total variance of $f(\mathbf{Z})$ decomposes as a sum of contributive parts. Moreover, given that these projections also satisfy the annihilating property (5), formulae (6) and (7) yield the same decomposition as a result of Proposition 2.

Turning to the Möbius decomposition introduced by Deheuvels [15] for testing mutual independence in a vector of continuous random variables, first note that one can limit the discussion to the class \mathcal{F} of d -variate copulas, i.e., d -variate cumulative distribution functions whose margins are uniform on the interval $[0, 1]$. This is because if X_1, \dots, X_d are random variables with continuous cumulative distribution functions F_1, \dots, F_d , respectively, mutual independence between them occurs if and only if the uniform random variables $Z_1 = F_1(X_1), \dots, Z_d = F_d(X_d)$ are mutually independent, i.e., their joint distribution, which is a copula, coincides with the independence copula, defined for all vectors $(z_1, \dots, z_d) \in D = [0, 1]^d$, by $\Pi(z_1, \dots, z_d) = z_1 \times \dots \times z_d$.

For arbitrary set $v \subseteq \{1, \dots, d\}$ and vector $\mathbf{x} = (x_1, \dots, x_d) \in [0, 1]^d$, let $\mathbf{x}_{v,1}$ denote the vector (t_1, \dots, t_d) such that $t_i = x_i$ if $i \in v$ and $t_i = 1$ otherwise. The Möbius decomposition of a copula C is then given, for all $\mathbf{x} \in [0, 1]^d$, by

$$C(\mathbf{x}) = \Pi(\mathbf{x}) + \sum_{u \subseteq \{1, \dots, d\}, |u| \geq 2} \mathcal{M}_u(C)(\mathbf{x}) \times \prod_{k \notin u} x_k, \quad (8)$$

where

$$\mathcal{M}_u(C)(\mathbf{x}) = \sum_{v \subseteq u} (-1)^{|u \setminus v|} C(\mathbf{x}_{v,1}) \times \prod_{k \in u \setminus v} x_k. \quad (9)$$

The restriction to a copula is actually unnecessary, as the identity extends to any cumulative distribution function whose support is $[0, 1]^d$; see Lemma 6 of [20].

Note that the definition (9) also makes sense for sets $u \subseteq \{1, \dots, d\}$ of cardinality 0 or 1, which yields $\mathcal{M}_u(C) = 1$ when $|u| = 0$ and $\mathcal{M}_u(C) = 0$ when $|u| = 1$. Therefore, formula (8) can be written alternatively, for all $\mathbf{x} \in [0, 1]^d$, as

$$C(\mathbf{x}) = \sum_{u \subseteq \{1, \dots, d\}} C_u(\mathbf{x})$$

with

$$C_u(\mathbf{x}) = \mathcal{M}_u(C)(\mathbf{x}) \times \prod_{k \notin u} x_k = \sum_{v \subseteq u} (-1)^{|u \setminus v|} C(\mathbf{x}_{v,1}) \times \prod_{k \notin v} x_k. \quad (10)$$

To see that this representation can be expressed in the form (1) with components defined through formula (2) in terms of commuting projections P_1, \dots, P_d , it suffices to define, for all $i \in \{1, \dots, d\}$, $C \in \mathcal{F}$, and $\mathbf{x} = (x_1, \dots, x_d) \in [0, 1]^d$,

$$P_i C(\mathbf{x}) = x_i \times C(x_1, \dots, x_{i-1}, 1, x_{i+1}, \dots, x_d). \quad (11)$$

The maps P_1, \dots, P_d so defined are clearly commuting projections, and it follows from their definition that for any set $v \subseteq \{1, \dots, d\}$ with $-v = \{1, \dots, d\} \setminus v$ and vector $\mathbf{x} \in [0, 1]^d$,

$$P_{-v} C(\mathbf{x}) = C(\mathbf{x}_{v,1}) \Pi(\mathbf{x}_{-v}).$$

It then follows from definition (10) that for every set $u \subseteq \{1, \dots, d\}$ and vector $\mathbf{x} \in [0, 1]^d$,

$$C_u(\mathbf{x}) = \sum_{v \subseteq u} (-1)^{|u \setminus v|} P_{-v} C(\mathbf{x}). \quad (12)$$

Observe that with projections of the form (11) with $i \in \{1, \dots, d\}$, the first term in the Möbius decomposition corresponds to the independence copula and that all first-order terms vanish. That is, for all $\mathbf{x} \in [0, 1]^d$, one has

$$C_{\emptyset}(\mathbf{x}) = P_{\{1, \dots, d\}} C(\mathbf{x}) = \Pi(\mathbf{x})$$

and for all $i \in \{1, \dots, d\}$,

$$\begin{aligned} C_{\{i\}}(\mathbf{x}) &= P_{\{1, \dots, d\} \setminus \{i\}}(C)(\mathbf{x}) - P_{\{1, \dots, d\}} C(\mathbf{x}) \\ &= C(\mathbf{x}_{\{i\}}) \Pi(\mathbf{x}_{\{1, \dots, d\} \setminus \{i\}}) - \Pi(\mathbf{x}) = 0. \end{aligned}$$

As it happens, however, Assumption 3 does not hold for the projections defined in (11). Nevertheless, the term (12) in the Möbius decomposition is consistent with representation (7). This suggests that Proposition 2 is valid in a slightly more general setting than covered by Theorem 2.1 of [22]. This point is developed next.

4. A slight extension

The following result relaxes Assumption 1 in Proposition 1 so that both the Hoeffding–Sobol and the Möbius decompositions can be derived from a common representation of multivariate functions. This generalization is stated below *in extenso* to facilitate external referencing. For internal consistency, however, the equation numbers appearing therein are repeated from their first occurrence above.

Proposition 3. *Let \mathcal{F} be a linear space of real-valued functions acting on a domain D of \mathbb{R}^d and let P_1, \dots, P_d be projections on \mathcal{F} which are commuting. Then, any function $f \in \mathcal{F}$ can be written in the form*

$$f = \sum_{u \subseteq \{1, \dots, d\}} f_u, \tag{1}$$

in which the term f_u , defined by

$$f_u = \left(\prod_{i \in u} (I_D - P_i) \prod_{i \notin u} P_i \right) (f), \tag{2}$$

is such that the annihilating property is satisfied, meaning that, for all $i \in \{1, \dots, d\}$,

$$P_i(f_u) = \begin{cases} 0 & \text{if } i \in u, \\ f_u & \text{if } i \notin u. \end{cases} \tag{5}$$

Moreover, if any function $f \in \mathcal{F}$ can be expressed as in (1) and the annihilating property (5) holds, then the term f_u is given by formula (2), which is equivalent to

$$f_u = P_{\{1, \dots, d\} \setminus u}(f) - \sum_{v \subsetneq u} f_v, \tag{6}$$

and to

$$f_u = \sum_{v \subseteq u} (-1)^{|u \setminus v|} P_{\{1, \dots, d\} \setminus v}(f), \tag{7}$$

where for any $u \subseteq \{1, \dots, d\}$, $P_u = \prod_{i \in u} P_i$.

Proof. To recover the desired decomposition, first call on the multinomial formula to see that

$$\prod_{i=1}^d I_D = \prod_{i=1}^d \{(I_D - P_i) + P_i\} = \sum_{u \subseteq \{1, \dots, d\}} \left(\prod_{i \in u} (I_D - P_i) \right) \left(\prod_{i \notin u} P_i \right)$$

with f_u defined as in (2). Accordingly, one finds

$$f = \left(\prod_{i=1}^d I_D \right) (f) = \sum_{u \subseteq \{1, \dots, d\}} \left(\prod_{i \in u} (I_D - P_i) \right) \left(\prod_{i \notin u} P_i \right) (f) = \sum_{u \subseteq \{1, \dots, d\}} f_u.$$

Furthermore, note that whatever $u \subseteq \{1, \dots, d\}$, the function f_u satisfies the annihilating property. Indeed, if $k \in u$, then

$$P_k(f_u) = \left(\prod_{i \in u \setminus \{k\}} (I_D - P_i) \right) \left(\prod_{i \notin u} P_i \right) P_k(I_D - P_k)(f) = 0$$

while if $k \notin u$, then

$$(I_D - P_k)(f_u) = \left(\prod_{i \in u} (I_D - P_i) \right) \left(\prod_{i \notin u, i \neq k} P_i \right) P_k(I_D - P_k)(f) = 0.$$

This proves the existence of the decomposition. To establish its uniqueness, write

$$f = \sum_{v \subseteq \{1, \dots, d\}} f_v,$$

and apply the projection P_{-u} . It follows from the annihilating property (5) that

$$P_{-u}(f) = \sum_{v \subseteq u} f_v = f_u + \sum_{v \subsetneq u} f_v,$$

which gives the recursive formula. Further note that $f_\emptyset = P_{\{1, \dots, d\}}(f)$ is a constant, as it should. Finally, formula (7) can be deduced from an expansion of the product formula, viz.

$$\begin{aligned} f_u &= \left(\prod_{i \in u} (I_D - P_i) \right) \left(\prod_{i \notin u} P_i \right) (f) \\ &= \sum_{v \subseteq u} (-1)^{|u \setminus v|} \left(\prod_{i \in u \setminus v} P_i \right) \left(\prod_{i \notin u} P_i \right) (f) = \sum_{v \subseteq u} (-1)^{|u \setminus v|} P_{-v}(f), \end{aligned}$$

70 which concludes the argument. □

71 In view of Proposition 3, the Möbius decomposition can thus be derived from projections and its terms can be
72 computed from (7) or equivalently from (2) or (6). This observation does not appear to have been documented
73 previously.

74 5. Discussion and perspectives

75 In the Hoeffding–Sobol decomposition, the projection P_u cancels the influence of variables in the subset u through
76 integration. The terms are of increasing complexity in the sense that f_u depends on \mathbf{x}_u , and the length of this
77 vector grows with the cardinality of u .

78 For the Möbius decomposition, the projection P_u erases the stochastic dependence between the variables whose
79 index is in the set u . More precisely, if a random vector \mathbf{Z} has distribution $P_u(C)$, the subvectors \mathbf{Z}_u and \mathbf{Z}_{-u}
80 are then independent. While there is no increasing complexity in the terms of the decomposition, given that
81 $C_u(\mathbf{x})$ depends on both \mathbf{x}_u and \mathbf{x}_{-u} , only the stochastic dependence embodied within \mathbf{x}_u is retained. It can be
82 said, therefore, that the terms in the Möbius decomposition are also increasing in complexity, but in the sense of
83 probabilistic dependence.

84 Beyond the relative degree of complexity of their terms, the Hoeffding–Sobol and Möbius decompositions each
85 have their comparative advantage. One key feature of the Hoeffding–Sobol decomposition is that it provides or-
86 thogonal terms, so that the structure of the function of interest can be analyzed through variances. In contrast, the
87 terms in the Möbius decomposition are not generally orthogonal. However, a strong point of the Möbius decompo-
88 sition is the ease with which any term can be of computed as a simple alternate combination of evaluations of the
89 function C .

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