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High dimensional model representations generated from low dimensional data samples. I. mp-Cut-HDMR

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High dimensional model representation (HDMR) is a general set of quantitative model assessment and analysis tools for improving the efficiency of deducing high dimensional input–output system behavior. For a high dimensional system, an output $f(\mathbf{x})$ is commonly a function of many input variables $\mathbf{x} = \{x_1, x_2, \ldots, x_n\}$ with $n \sim 10^2$ or larger. HDMR describes $f(\mathbf{x})$ by a finite hierarchical correlated function expansion in terms of the input variables. Various forms of HDMR can be constructed for different purposes. Cut- and RS-HDMR are two particular HDMR expansions. Since the correlated functions in an HDMR expansion are optimal choices tailored to $f(\mathbf{x})$ over the entire domain of $\mathbf{x}$, the high order terms (usually larger than second order, or beyond pair cooperativity) in the expansion are often negligible. When the approximations given by the first and the second order Cut-HDMR correlated functions are not adequate, this paper presents a *monomial based preconditioned* HDMR method to represent the higher order terms of a Cut-HDMR expansion by expressions similar to the lower order ones with monomial multipliers. The accuracy of the Cut-HDMR expansion can be significantly improved using preconditioning with a minimal number of additional input–output samples without directly invoking the determination of higher order terms. The mathematical foundations of monomial based preconditioned Cut-HDMR is presented along with an illustration of its applicability to an atmospheric chemical kinetics model.

1. Introduction

Many problems in science and engineering reduce to the need for finding an efficiently constructed map of the relationship between sets of high dimensional input and output system variables. For example, a key output variable of photochemical air quality simulation models is the peak ozone concentration in a region, and the input variables are the chemical, physical and radiative factors which effect the ozone concentration. The system may be described by a mathematical model (e.g., typically a set of differential equations), where the input variables might be specified initial and boundary conditions as well as functions residing in the model, and the output variables would be drawn from

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the solution to the model or a functional of the solution. The input–output behavior may also be based on observations in the laboratory or field where a mathematical model cannot readily be constructed for the system. In this case the input consists of the laboratory (control) variables and the output(s) is the observed system response. Regardless of the circumstances, the input is often very high dimensional with many variables even if the output is only a single quantity. We refer to the input variables collectively as $\mathbf{x} = \{x_1, x_2, \ldots, x_n\}$ with often $n \sim 10^2$–10^3 or more, and the output as $f(\mathbf{x})$. For simplicity in the remainder of the paper and without loss of generality, we shall refer to the system as a model regardless of whether it involves modeling, laboratory experiments or field studies.

An important point to understand is that without the possibility of simplification, the general high dimensional representation problems posed by many realistic systems are of exponential difficulty (i.e., the effort grows exponentially with dimension n). This comment may be understood from the simple consideration of attempting to deduce the input–output mapping via sampling by s points in each of the n input variables and performing the corresponding model runs. A full sampling therefore calls for $\sim s^n$ model runs, which would be clearly out of the question for many realistic cases (e.g., $s \sim 10$ and $n \sim 10^2$–10^3 or more). This view is generally overly pessimistic as evident from various Monte Carlo statistical analyses where typically far more modest numbers of computational runs or experiments are performed to achieve convergent results. Such behavior implies that a much more economic sampling may be sufficient.

A general set of quantitative model assessment and analysis tools, termed High Dimensional Model Representation (HDMR), have been introduced [1–4] for improving the efficiency of deducing high dimensional input–output system behavior. The concepts behind HDMR aim to capitalize on the latter observations that realistic physical systems generally do not call for an exponentially growing number of samples to prescribe their input–output relationships. As the effect of inputs upon the output can be independent and cooperative, it is natural to express the model output $f(\mathbf{x})$ as a finite hierarchical correlated function expansion in terms of the input variables:

$$\begin{aligned} f(\mathbf{x}) = f_0 &+ \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \leqslant i < j \leqslant n} f_{ij}(x_i, x_j) + \sum_{1 \leqslant i < j < k \leqslant n} f_{ijk}(x_i, x_j, x_k) \\ &+ \cdots + \sum_{1 \leqslant i_1 < \cdots < i_l \leqslant n} f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l}) + \cdots \\ &+ f_{12\ldots n}(x_1, x_2, \ldots, x_n), \end{aligned} \tag{1}$$

where f_0 is a constant representing the mean response to $f(\mathbf{x})$, and $f_i(x_i)$ gives the independent contribution to $f(\mathbf{x})$ by the ith input variable acting alone, $f_{ij}(x_i, x_j)$ gives the pair correlated contribution of the input variables x_i and x_j, etc. The last term $f_{12\ldots n}(x_1, x_2, \ldots, x_n)$ contains any residual nth correlated contributions of all input variables. The above HDMR expansion has a finite number of terms and is always exact. Other expansions have been suggested [5], but they commonly have an infinite number of terms and all the terms are some specified functions (e.g., Hermite polynomials). A critical feature of the HDMR expansion is that its component functions f_0, $f_i(x_i)$, $f_{ij}(x_i, x_j), \ldots$ are optimal choices tailored to $f(\mathbf{x})$ over the entire domain of $\mathbf{x}$, and the high order terms in the expansion are generally expected to be negligible. In order to appreciate the new features of HDMR introduced in this paper, a brief summary of the relevant aspects of HDMR will be given in the remainder of this section.

The basic conjecture underlying HDMR is that the component functions in equation (1) arising in typical real problems are not likely to exhibit high order l (e.g., a term like $f_{ij}(x_i, x_j)$ is of the second order, $l = 2$) cooperativity among the input variables such that the significant terms in the HDMR expansion are expected to satisfy the relation: $l \ll n$ for $n \gg 1$, i.e., very often the first or the second order approximation

$$f(\mathbf{x}) \approx f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \leqslant i < j \leqslant n} f_{ij}(x_i, x_j) \tag{2}$$

provides a satisfactory result for $f(\mathbf{x})$ in many high dimensional systems. Broad evidence from statistics supports this conjecture where it is rarely found that more than input variable covariance (i.e., variable pair cooperativity) significantly arises. HDMR attempts to exploit this observation to efficiently determine high dimensional input–output system mapping. The presence of only low order variable cooperativity does not necessarily imply a small set of significant variables nor does it limit the non-linear nature of the input–output relationship.

This valuable property of low order input cooperativity for high dimensional systems may be utilized only if a proper means for calculating the HDMR component functions can be found. In order to do so, optimal procedures were applied for the determination of the HDMR component functions. Various forms of HDMR have been considered with applications to several scientific problems [3,4,6–8]. This paper will focus on what has been referred to as Cut-HDMR where the variable space is sampled in an orderly fashion along low dimensional cuts (i.e., sub-volumes) centered at a chosen reference point $\bar{\mathbf{x}}$ in the space. The formulas determining the zeroth, first, second and third order component functions for Cut-HDMR in equation (1) are as follows:

$$f_0 = f(\bar{\mathbf{x}}), \tag{3}$$

$$f_i(x_i) = f\left(x_i, \bar{\mathbf{x}}^i\right) - f_0, \tag{4}$$

$$f_{ij}(x_i, x_j) = f\left(x_i, x_j, \bar{\mathbf{x}}^{ij}\right) - f_i(x_i) - f_j(x_j) - f_0, \tag{5}$$

$$\begin{aligned} f_{ijk}(x_i, x_j, x_k) = {} & f\left(x_i, x_j, x_k, \bar{\mathbf{x}}^{ijk}\right) - f_{ij}(x_i, x_j) - f_{ik}(x_i, x_k) \\ & - f_{jk}(x_j, x_k) - f_i(x_i) - f_j(x_j) - f_k(x_k) - f_0, \end{aligned} \tag{6}$$

where $\bar{\mathbf{x}}^i$, $\bar{\mathbf{x}}^{ij}$ and $\bar{\mathbf{x}}^{ijk}$ are respectively $\bar{\mathbf{x}}$ without elements $\bar{x}_i$; $\bar{x}_i, \bar{x}_j$; and $\bar{x}_i$, $\bar{x}_j$, $\bar{x}_k$. $f(\bar{\mathbf{x}})$ is the value of $f(\mathbf{x})$ at $\bar{\mathbf{x}}$; $f(x_i, \bar{\mathbf{x}}^i)$ is the model output with all variables evaluated at $\bar{\mathbf{x}}$ except for x_i, etc.

All the component functions of Cut-HDMR possess the property that they vanish whenever any input variable in these functions takes on its corresponding value in $\bar{\mathbf{x}}$:

$$f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l})\big|_{x_{i_s}=\bar{x}_{i_s}} = 0, \quad i_s \in \{i_1, i_2, \ldots, i_l\}, \tag{7}$$

and thus they are all mutually orthogonal under the definition

$$\begin{aligned} & f_{i_1 i_2 \ldots i_p}(x_{i_1}, x_{i_2}, \ldots, x_{i_p}) f_{j_1 j_2 \ldots j_q}(x_{j_1}, x_{j_2}, \ldots, x_{j_q})\big|_{x_{i_s}=\bar{x}_{i_s}} = 0, \\ & i_s \in \{i_1, i_2, \ldots, i_p\} \cup \{j_1, j_2, \ldots, j_q\}. \end{aligned} \tag{8}$$

The component functions (i.e., $f_i(x_i)$, $f_{ij}(x_i, x_j), \ldots$) of Cut-HDMR are typically provided numerically, at discrete values of the input variables x_i, $x_j, \ldots$ produced from sampling the output function $f(\mathbf{x})$ for employment on the right-hand side of equations (3)–(6). Thus, numerical data tables can be constructed for these component functions, and the value of $f(\mathbf{x})$ for an arbitrary point $\mathbf{x}$ can be determined from these tables by performing only low dimensional interpolation over $f_i(x_i)$, $f_{ij}(x_i, x_j), \ldots$.

The component functions f_0, $f_i(x_i)$, $f_{ij}(x_i, x_j), \ldots$ in Cut-HDMR have clear mathematical meaning which is especially evident when $f(\mathbf{x})$ can be expanded as a convergent Taylor series at the reference point $\bar{\mathbf{x}}$. In the discussion here and the analysis later in the paper, Taylor series considerations will only be used in a formal sense to better understand the nature of HDMR; indeed, the purpose of HDMR is to circumvent the need to use expressions with a growing or infinite number of terms. According to the definitions given in equations (3)–(6), it is easy to prove that $f_0 = f(\bar{\mathbf{x}})$, i.e., the constant term of the Taylor series; the first order function $f_i(x_i)$ is the sum of *all* the Taylor series terms which only contain the variable x_i, while the second order function $f_{ij}(x_i, x_j)$ is the sum of *all* the Taylor series terms which only contain variables x_i and x_j, etc. Therefore, each distinct component function of Cut-HDMR is composed of an infinite sub-class of the full multi-dimensional Taylor series, and the sub-classes do not overlap one another, which is the basis for the orthogonality of Cut-HDMR component functions. The orthogonality of the component functions in HDMR may generally be viewed from another perspective. The component functions of HDMR can be obtained through application of a suitably defined set of linear operators $\wp_0$, $\wp_i$ $(i = 1, 2, \ldots, n)$, $\wp_{ij}$ $(1 \leqslant i < j \leqslant n)$, $\wp_{ijk}$ $(1 \leqslant i < j < k \leqslant n), \ldots$:

$$\wp_0 f(\mathbf{x}) = f_0, \tag{9}$$

$$\wp_i f(\mathbf{x}) = f_i(x_i), \tag{10}$$

$$\wp_{ij} f(\mathbf{x}) = f_{ij}(x_i, x_j), \tag{11}$$

$$\wp_{ijk} f(\mathbf{x}) = f_{ijk}(x_i, x_j, x_k). \tag{12}$$

It has been proved that all the operators are commutative projection operators and they are mutually orthogonal to one another [1,2]. The basis for orthogonality of all the projectors simply comes from the fact that f_0, $f_i(x_i)$, $f_{ij}(x_i, x_j), \ldots$ do not overlap one another. Any set of commutative projectors generate a *distributive lattice* whose elements are obtained by all possible combinations (Boolean addition and multiplication) of the projectors in the set. Any operator $\wp_t$ in the lattice provides an approximation

$\wp_t f(\mathbf{x})$ to the function $f(\mathbf{x})$. In particular, the lattice has a unique *maximal* projector $\mathcal{M}$ which provides the algebraically best approximation to the functions in a linear space $\mathcal{F}$ composed of all n-variable functions $f(\mathbf{x})$ [9].

Each projector $\wp_t$ has its range Φ_t which is a subspace of the linear space $\mathcal{F}$. Any function $f(\mathbf{x}) \in \Phi_t$ is invariant upon the action of $\wp_t$, i.e.,

$$\wp_t f(\mathbf{x}) = f(\mathbf{x}) \quad \forall f(\mathbf{x}) \in \Phi_t. \tag{13}$$

This implies that upon the action of $\wp_t$ there is no error for any function $f(\mathbf{x}) \in \Phi_t$. The larger the range Φ_t is, the better approximation for $\mathcal{F}$ that $\wp_t$ produces. Two projectors $\wp_i$ and $\wp_j$ are mutually orthogonal, as stated by

$$\wp_i \wp_j = \wp_j \wp_i = 0.$$

This is equivalent to

$$\Phi_i \cap \Phi_j = 0.$$

The range of the maximal projector $\mathcal{M}$ for the lattice generated by the mutually commutative projectors $\{\wp_1, \wp_2, \ldots, \wp_N\}$ is the union of all the ranges Φ_t, i.e.,

$$\Phi_{\mathcal{M}} = \Phi_1 \cup \Phi_2 \cup \cdots \cup \Phi_N. \tag{14}$$

When the projectors are mutually orthogonal, $\Phi_i \cap \Phi_j = 0$ for all $i \neq j$, then

$$\Phi_{\mathcal{M}} = \Phi_1 + \Phi_2 + \cdots + \Phi_N, \tag{15}$$

which is the largest invariant subspace in $\mathcal{F}$ among the invariant subspaces produced by all projectors in the lattice. Therefore, the projector $\mathcal{M}$ provides the algebraically best approximation for $\mathcal{F}$ in the lattice. As more orthogonal projectors are retained in the set, then $\Phi_{\mathcal{M}}$ becomes larger and the resultant approximation obtained by its maximal projector $\mathcal{M}$ [9] becomes better.

For instance, if we choose the subset $\mathcal{S}_1 = \{\wp_0, \wp_i\ (i = 1, 2, \ldots, n)\}$ of the above mutually orthogonal projectors to generate a lattice, then its maximal projector is simply the sum of all these projectors:

$$\mathcal{M}_1 = \wp_0 + \sum_{i=1}^{n} \wp_i, \tag{16}$$

and the best approximation of $f(\mathbf{x}) \in \mathcal{F}$ by the projectors in this lattice is

$$\begin{aligned} f(\mathbf{x}) \approx \mathcal{M}_1 f(\mathbf{x}) &= \wp_0 f(\mathbf{x}) + \sum_{i=1}^{n} \wp_i f(\mathbf{x}) \\ &= f_0 + \sum_{i=1}^{n} f_i(x_i), \end{aligned} \tag{17}$$

which is called the first order HDMR approximation for $f(\mathbf{x})$. Similarly, for the subset $\mathcal{S}_2 = \{\wp_0, \wp_i\ (i = 1, 2, \ldots, n), \wp_{ij}\ (1 \leqslant i < j \leqslant n)\}$, the best approximation of $f(\mathbf{x})$ is given by

$$f(\mathbf{x}) \approx \mathcal{M}_2 f(\mathbf{x}) = \wp_0 f(\mathbf{x}) + \sum_{i=1}^{n} \wp_i f(\mathbf{x}) + \sum_{1 \leqslant i < j \leqslant n} \wp_{ij} f(\mathbf{x})$$
$$= f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \leqslant i < j \leqslant n} f_{ij}(x_i, x_j), \tag{18}$$

which is called the second order HDMR approximation for $f(\mathbf{x})$, etc.

As $\mathcal{S}_1$ is a subset of $\mathcal{S}_2$, and $\mathcal{M}_2$ is the maximal projector in the lattice generated by $\mathcal{S}_2$, then $\Phi_{\mathcal{M}_1} \subset \Phi_{\mathcal{M}_2}$ and $\mathcal{M}_2$ is better than $\mathcal{M}_1$, i.e., the second order approximation of HDMR is better than the first order one. In general, higher order HDMR approximations for $\mathcal{F}$ are always better than lower order HDMR approximations. This implies that adding a new orthogonal projector into a sum of orthogonal projectors always produces a new projector with the associated HDMR approximation having better accuracy.

As argued earlier, very often the high order HDMR terms are small thereby making low (i.e., first and second) order HDMR approximations satisfactory for practical purposes. However, in some cases the first or second order HDMR approximations may not provide satisfactory accuracy, and higher order HDMR approximations might have to be considered. For Cut-HDMR the higher order terms demand a polynomically increasing number of data samples. If the higher order component functions of Cut-HDMR can be approximately represented in a similar fashion as those for the zeroth, first and second order component functions, then higher order approximations of Cut-HDMR can be included without dramatically increasing the number of experiments or model runs as well as reducing computer storage requirements. One way to realize this concept is to represent a high order Cut-HDMR component function as a sum of preconditioned low order Cut-HDMR component functions. The preconditioning (i.e., the process of building in expected behavior) may be accomplished by multiplying each low order Cut-HDMR component function with a suitable known function of the remaining input variables. For instance, a third order Cut-HDMR component function $f_{ijk}(x_i, x_j, x_k)$ may be approximated as

$$\begin{aligned} f_{ijk}(x_i, x_j, x_k) \approx{}& \varphi_{ijk}(x_i, x_j, x_k)\bar{f}_0 + \varphi_{jk}(x_j, x_k)\bar{f}_i(x_i) \\ &+ \varphi_{ik}(x_i, x_k)\bar{f}_j(x_j) + \varphi_{ij}(x_i, x_j)\bar{f}_k(x_k) \\ &+ \varphi_k(x_k)\bar{f}_{ij}(x_i, x_j) + \varphi_j(x_j)\bar{f}_{ik}(x_i, x_k) \\ &+ \varphi_i(x_i)\bar{f}_{jk}(x_j, x_k), \end{aligned} \tag{19}$$

where $\varphi_i(x_i), \varphi_j(x_j), \ldots, \varphi_{ijk}(x_i, x_j, x_k)$ are appropriate known functions (e.g., the products of monomials $(x_i - b_i)$, $(x_j - b_j)$ and $(x_k - b_k)$ where the b's are constants), and $\bar{f}_0$, $\bar{f}_i(x_i), \ldots, \bar{f}_{jk}(x_j, x_k)$ are Cut-HDMR component functions for some given function $\bar{f}(\mathbf{x})$ related to $f(\mathbf{x})$. To determine the preconditioned Cut-HDMR component functions, we require that all the terms in equation (19) must be produced by mutually orthogonal projectors which are also orthogonal to the lower order projectors $\wp_0, \wp_i, \ldots, \wp_{jk}$ such that adding these new terms to the second order Cut-HDMR approximation will definitely improve its accuracy. When the functions $\{\varphi\}$ are monomial products, this approximation is referred to as *monomial* based *preconditioned* Cut-HDMR, or mp-Cut-HDMR. Its theoretical foundation and an illustrative application to an atmospheric chemical kinetics model are presented in this paper.

The paper is organized as follows. Section 2 introduces the principles of the mp-Cut-HDMR method. All the mathematical proofs underlying the method are in the appendix. In section 3, an atmospheric model is used for illustration. Finally, section 4 contains conclusions.

2. Principles of monomial based preconditioned Cut-HDMR

2.1. New orthogonal projectors

When $f(\mathbf{x})$ is approximated by the lth order Cut-HDMR at reference point $\mathbf{a}$, the error of this approximation is the residual

$$\begin{aligned} r_l(\mathbf{x}) = f(\mathbf{x}) - f_0 - \sum_{i=1}^{n} f_i(x_i) - \sum_{1\leqslant i<j\leqslant n} f_{ij}(x_i, x_j) - \cdots \\ - \sum_{1\leqslant i_1<\cdots<i_l\leqslant n} f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l}). \end{aligned} \tag{20}$$

As mentioned in section 1, $f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l})$ is the sum of all the Taylor series terms which only contain the variables $x_{i_1}, x_{i_2}, \ldots, x_{i_l}$ when $f(\mathbf{x})$ can be expanded as a convergent Taylor series at point $\mathbf{a}$. Since the collective Cut-HDMR component functions $f_{i_1 i_2 \ldots i_s}(x_{i_1}, x_{i_2}, \ldots, x_{i_s})$ $(s = 0, 1, \ldots, l)$ remove all the Taylor series terms of $f(\mathbf{x})$ with up to l variables, then $r_l(\mathbf{x})$ is only composed of the Taylor series terms containing more than l variables.

In order to explore the contribution of the next term beyond that contained in the HDMR expansion in equation (20) consider a subset I from the set of indices $\{1, 2, \ldots, n\}$, i.e.,

$$I = \{i_1, i_2, \ldots, i_m\} \subseteq \{1, 2, \ldots, n\}, \quad m = l + 1, \tag{21}$$

and let

$$\mathbf{x}_I = \{x_{i_1}, x_{i_2}, \ldots, x_{i_m}\}. \tag{22}$$

Then $r_l(\mathbf{x}_I, \mathbf{a}^I)$ (where $\mathbf{a}^I$ is the $\mathbf{a}$ without elements $\{a_{i_1}, a_{i_2}, \ldots, a_{i_m}\}$) is the value of the residual with all variables evaluated at $\mathbf{a}$ except of the elements in $\mathbf{x}_I$. Considering that $r_l(\mathbf{x})$ may be viewed as composed of products of $(x_i - a_i)$ $(i = 1, 2, \ldots, n)$, therefore

$r_l(\mathbf{x}_I, \mathbf{a}^I)$ only contains the Taylor series terms with the variables in $\mathbf{x}_I$. This implies that $r_l(\mathbf{x}_I, \mathbf{a}^I)$ is an mth order Cut-HDMR component function

$$r_l(\mathbf{x}_I, \mathbf{a}^I) = f_{i_1 i_2 \ldots i_m}(x_{i_1}, x_{i_2}, \ldots, x_{i_m}). \tag{23}$$

The goal is finding an approximation for equation (23) with a form similar to that in equation (19). In order to do so, it is convenient to write $r_l(\mathbf{x}_I, \mathbf{a}^I)$ as

$$r_l(\mathbf{x}_I, \mathbf{a}^I) = \varphi(\mathbf{x}_I) \frac{r_l(\mathbf{x}_I, \mathbf{a}^I)}{\varphi(\mathbf{x}_I)} = \varphi(\mathbf{x}_I) h_{lI}(\mathbf{x}_I, \mathbf{a}^I), \tag{24}$$

where $\varphi(\mathbf{x}_I)$ is some specified function. If $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ can be reliably represented by either the first or second order Cut-HDMR approximations about some suitable center, then $\varphi(\mathbf{x}_I) h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ will provide an approximation of $r_l(\mathbf{x}_I, \mathbf{a}^I)$ having a form similar to that in equation (19). In this process we may view $\varphi(\mathbf{x}_I)$ as a preconditioning function that extracts some characteristic behavior from $f_{i_1 i_2 \ldots i_m}(x_{i_1}, x_{i_2}, \ldots, x_{i_m})$ before subjecting it to a Cut-HDMR approximation of low order. When $\varphi(\mathbf{x}_I)$ is a product of monomials, i.e.,

$$\varphi(\mathbf{x}_I) = \prod_{s=1}^{m} (x_{i_s} - a_{i_s}), \tag{25}$$

$$h_{lI}(\mathbf{x}_I, \mathbf{a}^I) = \frac{r_l(\mathbf{x}_I, \mathbf{a}^I)}{\prod_{s=1}^{m} (x_{i_s} - a_{i_s})}, \tag{26}$$

the process is referred to as *monomial based preconditioning*. In the following treatment, we only consider monomial based preconditioning.

There is a family of residuals $r_l(\mathbf{x}_I, \mathbf{a}^I)$'s with each being a function of m variables in the Taylor series expansion of $f(\mathbf{x})$ when all possible I's are considered, i.e., for I and I', $r_l(\mathbf{x}_I, \mathbf{a}^I)$ and $r_l(\mathbf{x}_{I'}, \mathbf{a}^{I'})$ correspond to different sets of terms in the Taylor series. The residuals do not overlap one another, and they also do not overlap with the terms in the Taylor series representing the lower order component functions f_0, $f_i(x_i), \ldots,$ $f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l})$ because all these terms have already been removed from $r_l(\mathbf{x})$. The $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$'s also possess this property. Hence, it is possible to create new orthogonal projectors upon the $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$'s.

Now we consider approximating $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ by second order Cut-HDMR at a new reference point

$$\mathbf{b} = \{b_1, b_2, \ldots, b_n\}. \tag{27}$$

Approximation of $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ beyond second order could be considered, but practical evidence indicates that the present formulation is both simple and often quite satisfactory. To avoid a singularity in $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$, choose

$$b_i \neq a_i \quad \text{for all } i, \tag{28}$$

and set

$$\mathbf{b}_I = \{b_{i_1}, b_{i_2}, \ldots, b_{i_m}\}. \tag{29}$$

Then we have

$$\begin{aligned}
h_{lI}\big(\mathbf{x}_I, \mathbf{a}^I\big) &\approx \bar{f}_0 + \sum_{s=1}^{m} \bar{f}_{i_s}(x_{i_s}) + \sum_{1\leqslant r<s\leqslant m} \bar{f}_{i_r i_s}(x_{i_r}, x_{i_s}) \\
&= \frac{r_l(\mathbf{b}_I, \mathbf{a}^I)}{\prod_{s=1}^m (b_{i_s} - a_{i_s})} \\
&\quad + \sum_{s=1}^{m}\left[\frac{r_l(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I)}{(x_{i_s} - a_{i_s})\prod_{r=1, i_r\neq i_s}^m (b_{i_r} - a_{i_r})} - \frac{r_l(\mathbf{b}_I, \mathbf{a}^I)}{\prod_{r=1}^m (b_{i_r} - a_{i_r})}\right] \\
&\quad + \sum_{1\leqslant r<s\leqslant m}\left[\frac{r_l(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I)}{(x_{i_r} - a_{i_r})(x_{i_s} - a_{i_s})\prod_{t=1, i_t\neq i_r, i_s}^m (b_{i_t} - a_{i_t})}\right. \\
&\quad - \frac{r_l(x_{i_r}, \mathbf{b}_I^{i_r}, \mathbf{a}^I)}{(x_{i_r} - a_{i_r})\prod_{t=1, i_t\neq i_r}^m (b_{i_t} - a_{i_t})} - \frac{r_l(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I)}{(x_{i_s} - a_{i_s})\prod_{t=1, i_t\neq i_s}^m (b_{i_t} - a_{i_t})} \\
&\quad \left. + \frac{r_l(\mathbf{b}_I, \mathbf{a}^I)}{\prod_{t=1}^m (b_{i_t} - a_{i_t})}\right]. \qquad (30)
\end{aligned}$$

The resultant second order Cut-HDMR component functions for $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ are then multiplied by $\varphi(\mathbf{x}_I) = \prod_{s=1}^m (x_{i_s} - a_{i_s})$ in equation (24), which gives an approximate representation for the mth order component function

$$\begin{aligned}
&f_{i_1 i_2 \ldots i_m}(x_{i_1}, x_{i_2}, \ldots, x_{i_m}) \\
&\quad = r_l\big(\mathbf{x}_I, \mathbf{a}^I\big) \\
&\quad = \prod_{s=1}^m (x_{i_s} - a_{i_s}) h_{lI}\big(\mathbf{x}_I, \mathbf{a}^I\big) \\
&\quad \approx \prod_{s=1}^m \frac{(x_{i_s} - a_{i_s})}{(b_{i_s} - a_{i_s})} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&\qquad + \sum_{s=1}^m \left[\prod_{r=1, i_r\neq i_s}^m \frac{(x_{i_r} - a_{i_r})}{(b_{i_r} - a_{i_r})} r_l\big(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I\big) - \prod_{r=1}^m \frac{(x_{i_r} - a_{i_r})}{(b_{i_r} - a_{i_r})} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\right] \\
&\qquad + \sum_{1\leqslant r<s\leqslant m}\left[\prod_{t=1, i_t\neq i_r, i_s}^m \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I\big)\right. \\
&\qquad - \prod_{t=1, i_t\neq i_r}^m \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(x_{i_r}, \mathbf{b}_I^{i_r}, \mathbf{a}^I\big) - \prod_{t=1, i_t\neq i_s}^m \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I\big) \\
&\qquad \left. + \prod_{t=1}^m \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\right], \qquad (31)
\end{aligned}$$

where $\mathbf{b}_I^{i_t}$, $\mathbf{b}_I^{i_r i_s}$ are just $\mathbf{b}_I$ without elements b_{i_t}; b_{i_r}, b_{i_s}, respectively. When all possible choices of I are considered, the collective terms give an approximation for the $(l+1)$th order component functions of the Cut-HDMR to $f(\mathbf{x})$ without directly evaluating $f_{i_1 i_2 \ldots i_m}$ by the original formulation indicated in equations (3)–(6). This approximation is termed as the $(l+1)$th order mp-Cut-HDMR.

The resultant new functions appearing in the mp-Cut-HDMR may be obtained as the resultant action of a set of new operators $\widetilde{\wp}_0$, $\widetilde{\wp}_{i_s}$, $\widetilde{\wp}_{i_r i_s}$, i.e.,

$$r_l\big(\mathbf{x}_I, \mathbf{a}^I\big) \approx \left[\widetilde{\wp}_0 + \sum_{s=1}^{m} \widetilde{\wp}_{i_s} + \sum_{1 \leqslant r < s \leqslant m} \widetilde{\wp}_{i_r i_s}\right] f(\mathbf{x}), \tag{32}$$

where

$$\widetilde{\wp}_0 f(\mathbf{x}) = \tilde{f}_0 = \prod_{s=1}^{m} \frac{(x_{i_s} - a_{i_s})}{(b_{i_s} - a_{i_s})} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big), \tag{33}$$

$$\begin{aligned}\widetilde{\wp}_{i_s} f(\mathbf{x}) = \tilde{f}_{i_s} = {} & \prod_{r=1, i_r \neq i_s}^{m} \frac{(x_{i_r} - a_{i_r})}{(b_{i_r} - a_{i_r})} r_l\big(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I\big) \\ & - \prod_{r=1}^{m} \frac{(x_{i_r} - a_{i_r})}{(b_{i_r} - a_{i_r})} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big),\end{aligned} \tag{34}$$

$$\begin{aligned}\widetilde{\wp}_{i_r i_s} f(\mathbf{x}) = \tilde{f}_{i_r i_s} = {} & \prod_{t=1, i_t \neq i_r, i_s}^{m} \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I\big) \\ & - \prod_{t=1, i_t \neq i_r}^{m} \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(x_{i_r}, \mathbf{b}_I^{i_r}, \mathbf{a}^I\big) \\ & - \prod_{t=1, i_t \neq i_s}^{m} \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I\big) \\ & + \prod_{t=1}^{m} \frac{(x_{i_t} - a_{i_t})}{(b_{i_t} - a_{i_t})} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big).\end{aligned} \tag{35}$$

For an approximation to second order Cut-HDMR terms, $m = 3$ and $I = \{i_1, i_2, i_3\}$ we have

$$\begin{aligned}r_2\big(\mathbf{b}_I, \mathbf{a}^I\big) = {} & f\big(b_{i_1}, b_{i_2}, b_{i_3}, \mathbf{a}^{i_1 i_2 i_3}\big) - f\big(b_{i_1}, b_{i_2}, \mathbf{a}^{i_1 i_2}\big) \\ & - f\big(b_{i_1}, b_{i_3}, \mathbf{a}^{i_1 i_3}\big) - f\big(b_{i_2}, b_{i_3}, \mathbf{a}^{i_2 i_3}\big) \\ & + f\big(b_{i_1}, \mathbf{a}^{i_1}\big) + f\big(b_{i_2}, \mathbf{a}^{i_2}\big) + f\big(b_{i_3}, \mathbf{a}^{i_3}\big) - f(\mathbf{a}),\end{aligned} \tag{36}$$

$$\begin{aligned}r_2\big(x_{i_1}, \mathbf{b}_I^{i_1}, \mathbf{a}^I\big) = {} & f\big(x_{i_1}, b_{i_2}, b_{i_3}, \mathbf{a}^{i_1 i_2 i_3}\big) - f\big(x_{i_1}, b_{i_2}, \mathbf{a}^{i_1 i_2}\big) \\ & - f\big(x_{i_1}, b_{i_3}, \mathbf{a}^{i_1 i_3}\big) - f\big(b_{i_2}, b_{i_3}, \mathbf{a}^{i_2 i_3}\big) \\ & + f\big(x_{i_1}, \mathbf{a}^{i_1}\big) + f\big(b_{i_2}, \mathbf{a}^{i_2}\big) + f\big(b_{i_3}, \mathbf{a}^{i_3}\big) - f(\mathbf{a}),\end{aligned} \tag{37}$$

$$
\begin{aligned}
r_2\big(x_{i_1}, x_{i_2}, \mathbf{b}_I^{i_1 i_2}, \mathbf{a}^I\big) = {} & f\big(x_{i_1}, x_{i_2}, b_{i_3}, \mathbf{a}^{i_1 i_2 i_3}\big) - f\big(x_{i_1}, x_{i_2}, \mathbf{a}^{i_1 i_2}\big) \\
& - f\big(x_{i_1}, b_{i_3}, \mathbf{a}^{i_1 i_3}\big) - f\big(x_{i_2}, b_{i_3}, \mathbf{a}^{i_2 i_3}\big) \\
& + f\big(x_{i_1}, \mathbf{a}^{i_1}\big) + f\big(x_{i_2}, \mathbf{a}^{i_2}\big) + f\big(b_{i_3}, \mathbf{a}^{i_3}\big) - f(\mathbf{a}).
\end{aligned} \tag{38}
$$

For an approximation to third order Cut-HDMR terms, $m = 4$ and $I = \{i_1, i_2, i_3, i_4\}$ we have

$$
\begin{aligned}
r_3\big(\mathbf{b}_I, \mathbf{a}^I\big) = {} & f\big(b_{i_1}, b_{i_2}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_1 i_2 i_3 i_4}\big) - f\big(b_{i_1}, b_{i_2}, b_{i_3}, \mathbf{a}^{i_1 i_2 i_3}\big) \\
& - f\big(b_{i_1}, b_{i_2}, b_{i_4}, \mathbf{a}^{i_1 i_2 i_4}\big) - f\big(b_{i_1}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_1 i_3 i_4}\big) \\
& - f\big(b_{i_2}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_2 i_3 i_4}\big) + f\big(b_{i_1}, b_{i_2}, \mathbf{a}^{i_1 i_2}\big) + f\big(b_{i_1}, b_{i_3}, \mathbf{a}^{i_1 i_3}\big) \\
& + f\big(b_{i_1}, b_{i_4}, \mathbf{a}^{i_1 i_4}\big) + f\big(b_{i_2}, b_{i_3}, \mathbf{a}^{i_2 i_3}\big) + f\big(b_{i_2}, b_{i_4}, \mathbf{a}^{i_2 i_4}\big) \\
& + f\big(b_{i_3}, b_{i_4}, \mathbf{a}^{i_3 i_4}\big) - f\big(b_{i_1}, \mathbf{a}^{i_1}\big) - f\big(b_{i_2}, \mathbf{a}^{i_2}\big) \\
& - f\big(b_{i_3}, \mathbf{a}^{i_3}\big) - f\big(b_{i_4}, \mathbf{a}^{i_4}\big) + f(\mathbf{a}),
\end{aligned} \tag{39}
$$

$$
\begin{aligned}
r_3\big(x_{i_1}, \mathbf{b}_I^{i_1}, \mathbf{a}^I\big) = {} & f\big(x_{i_1}, b_{i_2}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_1 i_2 i_3 i_4}\big) - f\big(x_{i_1}, b_{i_2}, b_{i_3}, \mathbf{a}^{i_1 i_2 i_3}\big) \\
& - f\big(x_{i_1}, b_{i_2}, b_{i_4}, \mathbf{a}^{i_1 i_2 i_4}\big) - f\big(x_{i_1}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_1 i_3 i_4}\big) \\
& - f\big(b_{i_2}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_2 i_3 i_4}\big) + f\big(x_{i_1}, b_{i_2}, \mathbf{a}^{i_1 i_2}\big) + f\big(x_{i_1}, b_{i_3}, \mathbf{a}^{i_1 i_3}\big) \\
& + f\big(x_{i_1}, b_{i_4}, \mathbf{a}^{i_1 i_4}\big) + f\big(b_{i_2}, b_{i_3}, \mathbf{a}^{i_2 i_3}\big) + f\big(b_{i_2}, b_{i_4}, \mathbf{a}^{i_2 i_4}\big) \\
& + f\big(b_{i_3}, b_{i_4}, \mathbf{a}^{i_3 i_4}\big) - f\big(x_{i_1}, \mathbf{a}^{i_1}\big) - f\big(b_{i_2}, \mathbf{a}^{i_2}\big) \\
& - f\big(b_{i_3}, \mathbf{a}^{i_3}\big) - f\big(b_{i_4}, \mathbf{a}^{i_4}\big) + f(\mathbf{a}),
\end{aligned} \tag{40}
$$

$$
\begin{aligned}
r_3\big(x_{i_1}, x_{i_2}, \mathbf{b}_I^{i_1 i_2}, \mathbf{a}^I\big) = {} & f\big(x_{i_1}, x_{i_2}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_1 i_2 i_3 i_4}\big) - f\big(x_{i_1}, x_{i_2}, b_{i_3}, \mathbf{a}^{i_1 i_2 i_3}\big) \\
& - f\big(x_{i_1}, x_{i_2}, b_{i_4}, \mathbf{a}^{i_1 i_2 i_4}\big) - f\big(x_{i_1}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_1 i_3 i_4}\big) \\
& - f\big(x_{i_2}, b_{i_3}, b_{i_4}, \mathbf{a}^{i_1 i_2 i_3 i_4}\big) + f\big(x_{i_1}, x_{i_2}, \mathbf{a}^{i_1 i_2}\big) + f\big(x_{i_1}, b_{i_3}, \mathbf{a}^{i_1 i_3}\big) \\
& + f\big(x_{i_1}, b_{i_4}, \mathbf{a}^{i_1 i_4}\big) + f\big(x_{i_2}, b_{i_3}, \mathbf{a}^{i_2 i_3}\big) + f\big(x_{i_2}, b_{i_4}, \mathbf{a}^{i_2 i_4}\big) \\
& + f\big(b_{i_3}, b_{i_4}, \mathbf{a}^{i_3 i_4}\big) - f\big(x_{i_1}, \mathbf{a}^{i_1}\big) - f\big(x_{i_2}, \mathbf{a}^{i_2}\big) \\
& - f\big(b_{i_3}, \mathbf{a}^{i_3}\big) - f\big(b_{i_4}, \mathbf{a}^{i_4}\big) + f(\mathbf{a}).
\end{aligned} \tag{41}
$$

The formulas of $r_l(\mathbf{b}_I, \mathbf{a}^I)$, $r_l(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I)$ and $r_l(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I)$ for larger l can be readily produced. Similar to second order Cut-HDMR, only one- and two-dimensional look-up tables for $r_l(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I)$ and $r_l(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I)$ are needed for mp-Cut-HDMR taken to second order. This behavior greatly reduces the amount of samples needed to at least pick up a reasonable approximation to the terms beyond second order in the original Cut-HDMR expansion.

It can be proved (see the appendix) that all the operators $\widetilde{\wp}_0$, $\widetilde{\wp}_{i_s}$ and $\widetilde{\wp}_{i_r i_s}$ for a given m are mutually orthogonal projectors, and orthogonal to $\wp_0, \wp_i, \wp_{ij}, \ldots, \wp_{i_1 i_2 \ldots i_l}$ as well. Then the projectors $\{\wp\}$ of the lth order Cut-HDMR and the new projectors $\{\widetilde{\wp}\}$ of the

mth order mp-Cut-HDMR together generate a larger lattice. The maximal projector of the larger lattice is

$$\mathcal{M} = \wp_0 + \sum_{i=1}^{n} \wp_i + \sum_{1 \leqslant i<j \leqslant n} \wp_{ij} + \cdots + \sum_{1 \leqslant i_1 < \cdots < i_l \leqslant n} \wp_{i_1 i_2 \ldots i_l} + \sum_I \left[\widetilde{\wp}_0 + \sum_{s=1}^{m} \widetilde{\wp}_{i_s} + \sum_{1 \leqslant r<s \leqslant m} \widetilde{\wp}_{i_r i_s} \right] \tag{42}$$

and the best approximation of $f(\mathbf{x}) \in \mathcal{F}$ in the larger lattice is

$$\begin{aligned} \mathcal{M} f(\mathbf{x}) &= \wp_0 f(\mathbf{x}) + \sum_{i=1}^{n} \wp_i f(\mathbf{x}) + \sum_{1 \leqslant i<j \leqslant n} \wp_{ij} f(\mathbf{x}) + \cdots + \sum_{1 \leqslant i_1 < \cdots < i_l \leqslant n} \wp_{i_1 i_2 \ldots i_l} f(\mathbf{x}) \\ &\quad + \sum_I \left[\widetilde{\wp}_0 f(\mathbf{x}) + \sum_{s=1}^{m} \widetilde{\wp}_{i_s} f(\mathbf{x}) + \sum_{1 \leqslant r<s \leqslant m} \widetilde{\wp}_{i_r i_s} f(\mathbf{x}) \right] \\ &= f_0 + \sum_{i=1}^{n} f_i + \sum_{1 \leqslant i<j \leqslant n} f_{ij} + \cdots + \sum_{1 \leqslant i_1 < \cdots < i_l \leqslant n} f_{i_1 i_2 \ldots i_l} \\ &\quad + \sum_I \left[\tilde{f}_0 + \sum_{s=1}^{m} \tilde{f}_{i_s} + \sum_{1 \leqslant r<s \leqslant m} \tilde{f}_{i_r i_s} \right]. \end{aligned} \tag{43}$$

For a given m, $f(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I)$ and $f(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I)$ are invariant to the $\mathcal{M}$ given in equation (42) whenever the truncated Cut-HDMR has order $l = m - 1$ (see the appendix). However, the lth order Cut-HDMR can be approximated by the combination of the second order Cut-HDMR and the third to lth order mp-Cut-HDMR component functions. Then a new operator

$$\mathcal{M} = \wp_0 + \sum_{i=1}^{n} \wp_i + \sum_{1 \leqslant i<j \leqslant n} \wp_{ij} + \sum_{p=3}^{l+1} \sum_{I_p} \left[\widetilde{\wp}_0 + \sum_{s=1}^{p} \widetilde{\wp}_{i_s} + \sum_{1 \leqslant r<s \leqslant p} \widetilde{\wp}_{i_r i_s} \right] \tag{44}$$

and the corresponding expansion

$$\mathcal{M} f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f_i + \sum_{1 \leqslant i<j \leqslant n} f_{ij} + \sum_{p=3}^{l+1} \sum_{I_p} \left[\tilde{f}_0 + \sum_{s=1}^{p} \tilde{f}_{i_s} + \sum_{1 \leqslant r<s \leqslant p} \tilde{f}_{i_r i_s} \right] \tag{45}$$

may be used for the approximation of $f(\mathbf{x})$. Notice that all the terms in equation (45) are of zeroth, first and second orders. The approximation given by equation (45) can pick up the essential features of $(l + 1)$th order Cut-HDMR, and may even have an accuracy similar to that for the $(l + 1)$th order Cut-HDMR, but the sizes of its look-up tables are much smaller.

Table 1
The increasing numbers of one- and two-dimensional ranges by adding projectors $\{\widetilde{\wp}\}$.

m	$f(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I)$	$f(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I)$
3	$3C_n^3$	$3C_n^3$
4	$4C_n^4$	$6C_n^4$
5	$5C_n^5$	$10C_n^5$
m	mC_n^m	$C_m^2 C_n^m$

2.2. *Ranges of new projectors*

As proved before [1,2], the range of the lth order Cut-HDMR is

$$\Phi_{\{l\}} = \bigcup_{i=1}^{n} f\left(x_i, \mathbf{a}^i\right) \bigcup_{1\leqslant i<j\leqslant n} f\left(x_i, x_j, \mathbf{a}^{ij}\right) \bigcup_{1\leqslant i<j<k\leqslant n} \cdots \bigcup_{i_1 i_2 \ldots i_l} f\left(x_{i_1}, x_{i_2}, \ldots, x_{i_l}, \mathbf{a}^{i_1 i_2 \ldots i_l}\right). \tag{46}$$

When the new orthogonal projectors $\{\widetilde{\wp}\}$ of the mth order mp-Cut-HDMR component functions defined in section 2.1 are added to the lth order Cut-HDMR, a new range for each I

$$\Phi_{\{I\}} = \bigcup_{s=1}^{m} f\left(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I\right) \bigcup_{1\leqslant r<s\leqslant m} f\left(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I\right) \tag{47}$$

is added to $\Phi_{\{l\}}$ (see the appendix). The increments of the range for different m are given in table 1, where

$$C_n^m = \frac{n!}{m!(n-m)!}. \tag{48}$$

The significance of this table can be understood by considering a case when $n = 10$. The second order Cut-HDMR has 10 one variable functions $f(x_i, \mathbf{a}^i)$ and 45 two variable functions $f(x_i, x_j, \mathbf{a}^{ij})$. If we add in the new projectors of the third order ($m = 3$) mp-Cut-HDMR component functions, there are $10 + 3C_{10}^3 = 10 + 360$ one variable functions $f(x_i, \mathbf{a}^i)$ and $f(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I)$ and as well as $45 + 3C_{10}^3 = 45 + 360$ two variable functions $f(x_i, x_j, \mathbf{a}^{ij})$ and $f(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I)$ for all possible I. These additional functions composed to new lines and planes through the $n = 10$ dimensional space upon which the function $f(\mathbf{x})$ is exactly represented. Thus, the accuracy of the modified second order Cut-HDMR can be dramatically improved (see section 3 below).

Compared to directly using higher order Cut-HDMR, the mp-Cut-HDMR needs smaller tables (i.e., fewer samples). As an example, suppose that each variable is sampled at s values. The total sampling for mth order component functions of

Cut-HDMR is $C_n^m s^m$, but the mth order mp-Cut-HDMR component functions only need $C_n^m(ms + C_m^2 s^2)$ samples. The ratio is

$$R = \frac{\text{Sampling of component functions of } m\text{th order mp-Cut-HDMR}}{\text{Sampling of } m\text{th order component functions of Cut-HDMR}}$$
$$= \frac{C_n^m(ms + C_m^2 s^2)}{C_n^m s^m} = \frac{m + C_m^2 s}{s^{m-1}}, \tag{49}$$

which is independent of n. For $m = 3$ and $s = 10$, $R \approx 1/3$. For $m = 5$ and $s = 10$, $R \approx 1/100$. The saving is obvious.

3. Example: A photochemical box model

A zero-dimensional photochemical box model designed to treat the ozone chemistry in the background troposphere is being used to study three-dimensional global chemical transport [7]. This box model consists of 63 reactions and 28 chemical species. Using this box model the rates of ozone production P and destruction D may be calculated and incorporated into the overall model. The details of this process [7] are not relevant here, but the box model provides a good testing ground for mp-Cut-HDMR. The rates of ozone production P and destruction D are used as two output variables of the box model. The input variables are month, latitude, altitude and the concentrations of 4 precursors: H_2O, CO, NO_x and O_3.

A tremendous amount of computational time would have to be spent to obtain the chemical ozone production and destruction rates by directly solving the associated differential equations at each time step of the three-dimensional model simulations. One promising solution to lift this computational burden is to employ Cut-HDMR expansions. The application of the second order Cut-HDMR for the input–output relationships of chemical kinetics was successful in a three-dimensional global chemistry-transport model study [7], with input variables as the concentrations of 4 precursors: H_2O, CO, NO_x and O_3 (the other three input variables were fixed) and two output variables: P and D. When the variables other than chemistry (i.e., month, latitude and altitude) are included as input variables, the accuracy of the second order Cut-HDMR was not satisfactory. In this paper, we will show that mp-Cut-HDMR can provide much better accuracy. In the following example, 5 input variables (month and 4 precursor concentrations: H_2O, CO, NO_x, O_3) with two output variables P and D are included. The input variable of *month* can effectively account for the role of temperature on the chemical rates of ozone production and destruction. The box is specified by 61.5°S latitude and 990 mb pressure.

Second and third order Cut-HDMR's were constructed for this 5 input and 2 output variable model. The mp-Cut-HDMR component functions with $m = 3, 4, 5$ were also constructed. The Cut-HDMR and mp-Cut-HDMR tables use the same ranges and

Table 2
The variable ranges and meshes of Cut-HDMR and mp-Cut-HDMR tables.

	Mesh spacing	Range	
		Lower limit	Upper limit
Month	1	1	12
Relative humidity (%)	5	5	100
CO (ppb)	10	10	200
NO_x (ppt)	50	50	750
O_3 (ppb)	10	10	150

Table 3
Comparison of the accuracy for Cut-HDMR and mp-Cut-HDMR.[a]

	Relative error					
	1%		5%		10%	
	P	*D*	*P*	*D*	*P*	*D*
2nd Cut-HDMR	18	24	44	50	59	63
2nd Cut-HDMR +						
3rd mp-Cut-HDMR	47	70	75	90	84	95
3rd, 4th mp-Cut-HDMR	65	81	87	95	92	98
3rd, 4th, 5th mp-Cut-HDMR	67	82	87	95	92	98
3rd Cut-HDMR	55	76	80	92	88	96
3rd Cut-HDMR +						
4th mp-Cut-HDMR	75	88	93	97	96	99
4th, 5th mp-Cut-HDMR	77	89	93	97	97	99

[a] The percentage of data with relative error not larger than a given value. The results of mp-Cut-HDMR are obtained by using equation (45).

sampling meshes for all input variables shown in table 2. The reference points **a** and **b** are chosen as follows:

$$\mathbf{a} = \{6, 65, 120, 450, 70\}, \qquad \mathbf{b} = \{9, 35, 60, 200, 40\}. \tag{50}$$

Point **a** is near the middle of the domain and point **b** is arbitrarily picked.

A set of 25,600 exact data obtained by solving the differential equations of the box model was compared to the approximate solutions given by Cut-HDMR and mp-Cut-HDMR. The test data were constructed by using the ranges listed in table 2, and some of the meshes used to construct the test data are larger, but all are contained in the meshes of table 2. Thus, there is no interpolation error when Cut-HDMR and mp-Cut-HDMR look-up tables are used. All the errors of Cut-HDMR and mp-Cut-HDMR come from the expansion truncation inherent with the method. For comparison, the percentages of the test data with relative errors not larger than 1, 5 and 10% for the two methods are shown in table 3.

From table 3, one can see that the accuracy of the second order Cut-HDMR is quite poor; only 44% and 50% of the data for chemical ozone production and destruc-

Table 4
The comparison between input data table sizes of Cut-HDMR and mp-Cut-HDMR.

	Relative size	
	To 2nd Cut-HDMR	To 3rd Cut-HDMR
2nd Cut-HDMR	1.000	0.035
2nd Cut-HDMR +		
3rd mp-Cut-HDMR	4.033	0.143
3rd, 4th mp-Cut-HDMR	7.015	0.249
3rd, 4th, 5th mp-Cut-HDMR	8.000	0.284
3rd Cut-HDMR	28.189	1.000
3rd Cut-HDMR +		
4th mp-Cut-HDMR	31.171	1.106
4th, 5th mp-Cut-HDMR	32.156	1.141

tion rates have relative error less than 5%. However, the combination of the second order Cut-HDMR with the third and fourth, or the third, fourth and fifth order mp-Cut-HDMR component functions have 87%, 95% data for chemical ozone production and destruction rates, respectively. The accuracy has been dramatically improved. The results are even better than the accuracy of the third order Cut-HDMR while the table sizes (i.e., the number of model runs necessary to determine the mp-Cut-HDMR) are only about 1/4 of the third order Cut-HDMR table (see table 4). The same tendency can be found for other relative errors.

The behavior in table 3 also reflects the orthogonality of the mp-Cut-HDMR component functions with different order m. In the appendix, we only prove that the component functions of mth (i.e., $(l+1)$th) order mp-Cut-HDMR are orthogonal to one another, and to all component functions of lth order Cut-HDMR. When the lth order Cut-HDMR are approximately represented as the combination of the second order Cut-HDMR and the third to lth order mp-Cut-HDMR component functions, the mutual orthogonality between all the functions of second order Cut-HDMR and different order mp-Cut-HDMR has not been proved, yet. They may not be exactly mutually orthogonal. However, the results in table 3 show that the accuracy is always improved whenever a higher order mp-Cut-HDMR component function is added, i.e., they appear to be mutually orthogonal. Moreover, compared to $m = 5$, the mp-Cut-HDMR component functions with $m = 3, 4$ add more one- and two-dimensional invariant ranges (see table 1) in this 5 input variable model, they improve the accuracy more. These results show that higher order component functions of Cut-HDMR are effectively approximated by mp-Cut-HDMR component functions.

The accuracy for both Cut-HDMR and mp-Cut-HDMR can depend on the choice of the reference points **a** and **b**. As a simple test of this issue, we interchanged **a** and **b**, and the results are given in table 5.

The point **a** is located near the center of the domain for the 5 input variables. Thus, the corresponding second order Cut-HDMR has a better accuracy compared to using **b** as the reference point. However, interchanging the **a** and **b** does not change the tendency

Table 5
The comparison of the accuracy for Cut-HDMR and mp-Cut-HDMR.[a]

	Relative error					
	1%		5%		10%	
	P	*D*	*P*	*D*	*P*	*D*
2nd Cut-HDMR	9	14	25	33	37	45
2nd Cut-HDMR +						
3rd mp-Cut-HDMR	36	47	62	75	70	83
3rd, 4th mp-Cut-HDMR	50	69	74	88	79	94
3rd, 4th, 5th mp-Cut-HDMR	56	82	86	95	92	98

[a] The percentage of data with relative error not larger than a given value. The points **a** and **b** are interchanged.

for improvement provided by mp-Cut-HDMR. Especially, when 3rd + 4th + 5th mp-Cut-HDMR component functions are used, the accuracies are almost identical for the two cases upon comparing tables 3 and 5. As the test system has dimension 5, the third, fourth and fifth order mp-Cut-HDMR contains the approximations of all order residuals $r_l(\mathbf{x})$ $(l = 3, 4, 5)$. When the system dimension n is high, we may not approximate all order residuals by mp-Cut-HDMR. Only low order mp-Cut-HDMR component functions $(l \ll n)$ are practical for construction, and the proper choice of **a** and **b** can be important.

4. Conclusions

This paper presents a monomial based approach to approximately represent the high order component functions of Cut-HDMR. The operating formulas of mp-Cut-HDMR are similar to the lower order component functions of Cut-HDMR with monomial multipliers. The resultant approximate expressions of the higher order component functions are then added to the original truncated lower order Cut-HDMR. The accuracy is guaranteed to improve because the new functions are produced by projectors which are mutually orthogonal including to the original projectors generating the truncated lower order Cut-HDMR. The amount of data needed to generate the mp-Cut-HDMR component functions is much smaller than that required for higher order Cut-HDMR, and the mp-Cut-HDMR gives better accuracy.

A subsystem with five input and two output variables of a photochemical box model was used for illustration of mp-Cut-HDMR. The mp-Cut-HDMR dramatically improves the accuracy of the lower order Cut-HDMR. The accuracy was shown to always improve whenever a higher order mp-Cut-HDMR component function is added. The combination of the second order Cut-HDMR with the third and fourth, or the third, fourth and fifth order mp-Cut-HDMR component functions has an accuracy even better than the third order Cut-HDMR, but the amount of data needed is only $\sim$1/4 of that required by the third order Cut-HDMR. These results show that higher order component functions of Cut-HDMR are effectively approximated by mp-Cut-HDMR component functions.

The orthogonality of the mp-Cut-HDMR component functions is the key to its success. Their orthogonality comes from two factors. First, the expansion terms for $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ are related to the sum of *all* the terms in the Taylor series of $f(\mathbf{x})$ involving the variables $x_{i_1}, x_{i_2}, \ldots, x_{i_m}$. This guarantees that all the expansion terms of $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ do not overlap one another for different I and m, and as well as do not overlap with all the terms producing the lower order Cut-HDMR. This is a basis for all the component functions of mp-Cut-HDMR being produced by mutually orthogonal projectors.

Monomial based preconditioning also has special orthogonality features. If the expansion of $h_{lI}(\mathbf{x}_I, \mathbf{a}^I)$ is exact, the division and multiplication of $\prod_{s=1}^{m}(x_{i_s} - a_{i_s})$ will cancel each other, and the expansion is equivalent to the expansion of $r_l(\mathbf{x}_I, \mathbf{a}^I)$. Although the expansion of $r_l(\mathbf{x}_I, \mathbf{a}^I)$ is truncated, nevertheless it is a good approximate representation of $r_l(\mathbf{x}_I, \mathbf{a}^I)$. If we directly expand $r_l(\mathbf{x}_I, \mathbf{a}^I)$ to second order Cut-HDMR, these terms are not orthogonal to the component functions of lth order Cut-HDMR. For instance, when $\mathbf{x} = \{x_i, \mathbf{a}^i\}$, and $f_0(\mathbf{a}) + f_i(x_i, \mathbf{a}^i)$ gives the exact solution for $f(x_i, \mathbf{a}^i)$, then the other terms should be zero. Unfortunately, $\bar{f}_0$ in the direct expansion of $r_l(\mathbf{x}_I, \mathbf{a}^I)$ is a constant and never vanishes. However, $\prod_{s=1}^{m}(x_{i_s} - a_{i_s})$ will make $\tilde{f}_0$ vanish if mp-Cut-HDMR is used because $\prod_{s=1}^{m}(x_{i_s} - a_{i_s}) = 0$ at $\{x_i, \mathbf{a}^i\}$. The monomial $\prod_{s=1}^{m}(x_{i_s} - a_{i_s})$ is not the only choice for this purpose. Other functions $\varphi(\mathbf{x}_I)$ can be considered, but they must have roots at $x_{i_s} = a_{i_s}$ $(s = 1, 2, \ldots, m)$.

The considerations underlying mp-Cut-HDMR are based on the existence of a convergent Taylor series for $f(\mathbf{x})$ around a single reference point $\mathbf{a}$. mp-Cut-HDMR provides approximations of the remaining terms after those corresponding to lth order Cut-HDMR have been removed. The assumption behind this treatment is that the Taylor expansion is convergent in the domain of $\mathbf{x}$ under consideration. If this assumption is not satisfied, one can divide the domain into sub-domains. Within each sub-domain a convergent Taylor series for $f(\mathbf{x})$ may be constructed. If the lth order Cut-HDMR does not have satisfactory accuracy in this sub-domain, then mp-Cut-HDMR may be employed to improve the accuracy. For the whole domain there may be several Taylor series of $f(\mathbf{x})$ around distinct reference points in different sub-domains. We refer to this method as *multi* Cut-HDMR. The key point for multi Cut-HDMR is that the projectors corresponding to all sub-domains are mutually orthogonal so that the sum of all the projectors compose the maximal projector $\mathcal{M}$, and $\mathcal{M}f(\mathbf{x})$ gives the best approximation of $f(\mathbf{x}) \in \mathcal{F}$ in the whole domain. This perspective will be developed in future work.

Appendix

The treatment below will prove that the component functions generated by mth order mp-Cut-HDMR are all produced by commutative projectors $\{\widetilde{\wp}\}$ orthogonal to all the original projectors of lth order Cut-HDMR and to one another. To simplify the formulas, the subscripts i_r, i_s may be replaced by i and j in the following proofs.

The new operators $\{\widetilde{\wp}\}$ of mp-Cut-HDMR contain the following terms:

$$\prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big),\qquad \prod_{s=1,i_s\neq i}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big),$$

$$\prod_{s=1,i_s\neq i,j}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I\big).$$

When more than $n-m$ elements of $\mathbf{x}$ take on values of the corresponding elements of $\mathbf{a}$, then at least one case of $x_{i_s}=a_{i_s}$ occurs either in the products $\prod_{s=1}^{m}(x_{i_s}-a_{i_s})/(b_{i_s}-a_{i_s})$, $\prod_{s=1,i_s\neq i}^{m}(x_{i_s}-a_{i_s})/(b_{i_s}-a_{i_s})$ and $\prod_{s=1,i_s\neq i,j}^{m}(x_{i_s}-a_{i_s})/(b_{i_s}-a_{i_s})$ or in the residual functions of lth order Cut-HDMR $r_l(x_i,\mathbf{b}_I^i,\mathbf{a}^I)$ and $r_l(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I)$. In this case, either the products are zero, or the lth order residual vanishes because the lth order residual is zero for all the points $\mathbf{x}$ with more than $n-m$ elements taking on the corresponding values of $\mathbf{a}$. Then all the three terms vanish. This property will be implicitly used in the following proofs.

A.1. Projection operator idempotency

We will prove that the operators $\widetilde{\wp}_0$ $\widetilde{\wp}_i$, $(i=1,2,\ldots,n)$ and $\widetilde{\wp}_{ij}$ $(1\leqslant i<j\leqslant n)$ defined in equations (33)–(35) for $m=3,4,\ldots,n$ possess the property of idempotency, and hence they are projectors.

1. $\widetilde{\wp}_0$

$$\widetilde{\wp}_0\widetilde{\wp}_0 f(\mathbf{x})=\widetilde{\wp}_0\left[\prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\right].\tag{A.1}$$

Notice that in equation (A.1) $\widetilde{\wp}_0$ acts on $\prod_{s=1}^{m}[(x_{i_s}-a_{i_s})/(b_{i_s}-a_{i_s})]r_l(\mathbf{b}_I,\mathbf{a}^I)$ which is the function $f(\mathbf{x})$ in equation (33). Then using equation (20) a new $r_l(\mathbf{b}_I,\mathbf{a}^I)$ should be calculated for $f(\mathbf{x})=\prod_{s=1}^{m}[(x_{i_s}-a_{i_s})/(b_{i_s}-a_{i_s})]r_l(\mathbf{b}_I,\mathbf{a}^I)$. Considering the property mentioned at the beginning of the appendix, all the terms except the first one of the new $r_l(\mathbf{b}_I,\mathbf{a}^I)$ have more than $n-m$ coordinates taking on the corresponding values of $\mathbf{a}$ and then they vanish. Thus, we have

$$\widetilde{\wp}_0\widetilde{\wp}_0 f(\mathbf{x})=\prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)=\widetilde{\wp}_0 f(\mathbf{x}).\tag{A.2}$$

As $f(\mathbf{x})$ is arbitrary, this implies that

$$\widetilde{\wp}_0\widetilde{\wp}_0=\widetilde{\wp}_0.\tag{A.3}$$

2. $\widetilde{\wp}_i$

$$\widetilde{\wp}_i\widetilde{\wp}_i f(\mathbf{x}) = \widetilde{\wp}_i\left[\prod_{s=1,i_s\neq i}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big) - \prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\right]. \tag{A.4}$$

Similarly, $\widetilde{\wp}_i$ acting on each of the two terms gives

$$\begin{aligned}\widetilde{\wp}_i\widetilde{\wp}_i f(\mathbf{x}) &= \prod_{s=1,i_s\neq i}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big) - \prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\\ &\quad - \prod_{s=1,i_s\neq i}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}\left[\frac{x_i-a_i}{b_i-a_i}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\right] + \prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\\ &= \prod_{s=1,i_s\neq i}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big) - \prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\\ &= \widetilde{\wp}_i f(\mathbf{x}).\end{aligned} \tag{A.5}$$

Here the relation

$$\prod_{s=1,i_s\neq i}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}\left(\frac{x_i-a_i}{b_i-a_i}\right) = \prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} \tag{A.6}$$

was used. This implies that

$$\widetilde{\wp}_i\widetilde{\wp}_i = \widetilde{\wp}_i. \tag{A.7}$$

In the proof we had an additional result from the last term of equation (A.4)

$$\widetilde{\wp}_i\prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big) = \widetilde{\wp}_i\widetilde{\wp}_0 f(\mathbf{x}) = 0, \tag{A.8}$$

i.e.,

$$\widetilde{\wp}_i\widetilde{\wp}_0 = 0. \tag{A.9}$$

3. $\widetilde{\wp}_{ij}$

Following the same procedure we have

$$\begin{aligned}\widetilde{\wp}_{ij}\widetilde{\wp}_{ij} f(\mathbf{x}) = \widetilde{\wp}_{ij}\Bigg[&\prod_{s=1,i_s\neq i,j}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I\big)\\ &- \prod_{s=1,i_s\neq i}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big) - \prod_{s=1,i_s\neq j}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(x_j,\mathbf{b}_I^j,\mathbf{a}^I\big)\\ &+ \prod_{s=1}^{m}\frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\Bigg].\end{aligned} \tag{A.10}$$

Using equation (35) we will treat each term in above equation one-by-one.

$$\begin{aligned}
&\widetilde{\wp}_{ij}\left[\prod_{s=1, i_s\neq i,j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big)\right] \\
&\quad= \prod_{s=1, i_s\neq i,j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) - \prod_{s=1, i_s\neq i}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \\
&\qquad - \prod_{s=1, i_s\neq j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_j, \mathbf{b}_I^{j}, \mathbf{a}^I\big) + \prod_{s=1}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&\quad= \widetilde{\wp}_{ij} f(\mathbf{x}).
\end{aligned} \tag{A.11}$$

$$\begin{aligned}
&\widetilde{\wp}_{ij}\left[\prod_{s=1, i_s\neq i}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big)\right] \\
&\quad= \prod_{s=1, i_s\neq i,j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} \left[\frac{x_j-a_j}{b_j-a_j} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big)\right] - \prod_{s=1, i_s\neq i}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \\
&\qquad - \prod_{s=1, i_s\neq j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} \left[\frac{x_j-a_j}{b_j-a_j} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\right] + \prod_{s=1}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&\quad= \prod_{s=1, i_s\neq i}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) - \prod_{s=1, i_s\neq i}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \\
&\qquad - \prod_{s=1}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) + \prod_{s=1}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) = 0.
\end{aligned} \tag{A.12}$$

Here the relation

$$\prod_{s=1, i_s\neq i,j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} \left(\frac{x_j-a_j}{b_j-a_j}\right) = \prod_{s=1, i_s\neq i}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} \tag{A.13}$$

and equation (A.6) were used. Similarly, we have

$$\widetilde{\wp}_{ij}\left[\prod_{s=1, i_s\neq j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_j, \mathbf{b}_I^{j}, \mathbf{a}^I\big)\right] = 0. \tag{A.14}$$

Finally, we have

$$\begin{aligned}
&\widetilde{\wp}_{ij}\left[\prod_{s=1}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\right] \\
&\quad= \widetilde{\wp}_{ij}\widetilde{\wp}_0 f(\mathbf{x})
\end{aligned}$$

$$
\begin{aligned}
&= \prod_{s=1, i_s \neq i,j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{(x_i - a_i)(x_j - a_j)}{(b_i - a_i)(b_j - a_j)} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] \\
&\quad - \prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_i - a_i}{b_i - a_i} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] - \prod_{s=1, i_s \neq j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_j - a_j}{b_j - a_j} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] \\
&\quad + \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&= \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \big[r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) + r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \big] = 0. \qquad \text{(A.15)}
\end{aligned}
$$

Here the relation

$$
\prod_{s=1, i_s \neq i,j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{(x_i - a_i)(x_j - a_j)}{(b_i - a_i)(b_j - a_j)} \right] = \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \qquad \text{(A.16)}
$$

and equation (A.6) were used.

Alltogether, we have

$$
\widetilde{\wp}_{ij} \widetilde{\wp}_{ij} f(\mathbf{x}) = \widetilde{\wp}_{ij} f(\mathbf{x}), \qquad \text{(A.17)}
$$

i.e.,

$$
\widetilde{\wp}_{ij} \widetilde{\wp}_{ij} = \widetilde{\wp}_{ij}. \qquad \text{(A.18)}
$$

As the second and the last terms, and the last two terms in equation (A.10) comprise $\widetilde{\wp}_i f(\mathbf{x})$ and $\widetilde{\wp}_j f(\mathbf{x})$, we have additionally

$$
\widetilde{\wp}_{ij} \widetilde{\wp}_i = \widetilde{\wp}_{ij} \widetilde{\wp}_j = \widetilde{\wp}_{ij} \widetilde{\wp}_0 = 0. \qquad \text{(A.19)}
$$

The above demonstrations collectively prove that the set of operators $\widetilde{\wp}_0$, $\widetilde{\wp}_i$ and $\widetilde{\wp}_{ij}$ are projectors.

A.2. Projection operator orthogonality

A.2.1. Orthogonality of $\{\widetilde{\wp}\}$ within each I

1. $\widetilde{\wp}_0$

In appendix A.1 we obtained $\widetilde{\wp}_{ij} \widetilde{\wp}_0 = \widetilde{\wp}_i \widetilde{\wp}_0 = 0$. Now, we only need to prove that $\widetilde{\wp}_0 \widetilde{\wp}_{ij} = \widetilde{\wp}_0 \widetilde{\wp}_i = 0$.

$$
\begin{aligned}
\widetilde{\wp}_0 \widetilde{\wp}_{ij} f(\mathbf{x}) = \widetilde{\wp}_0 \Bigg[&\prod_{s=1, i_s \neq i,j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) - \prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \\
&- \prod_{s=1, i_s \neq j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_j, \mathbf{b}_I^{j}, \mathbf{a}^I\big) + \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \Bigg]
\end{aligned}
$$

$$= \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[r_l\left(\mathbf{b}_I, \mathbf{a}^I\right) - r_l\left(\mathbf{b}_I, \mathbf{a}^I\right) - r_l\left(\mathbf{b}_I, \mathbf{a}^I\right) + r_l(\mathbf{b}_I, \mathbf{a}^I)\right] = 0.$$

$$\widetilde{\wp}_0 \widetilde{\wp}_i f(\mathbf{x}) = \widetilde{\wp}_0 \left[\prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\left(x_i, \mathbf{b}_I^i, \mathbf{a}^I\right) - \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\left(\mathbf{b}_I, \mathbf{a}^I\right) \right]$$

$$= \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[r_l\left(\mathbf{b}_I, \mathbf{a}^I\right) - r_l\left(\mathbf{b}_I, \mathbf{a}^I\right)\right] = 0. \tag{A.20}$$

Then we have

$$\widetilde{\wp}_0 \widetilde{\wp}_{ij} = \widetilde{\wp}_{ij} \widetilde{\wp}_0 = 0, \tag{A.21}$$

$$\widetilde{\wp}_0 \widetilde{\wp}_i = \widetilde{\wp}_i \widetilde{\wp}_0 = 0. \tag{A.22}$$

2. $\widetilde{\wp}_i$

We only need to prove that $\widetilde{\wp}_i \widetilde{\wp}_j = \widetilde{\wp}_j \widetilde{\wp}_i = \widetilde{\wp}_i \widetilde{\wp}_{ij} = \widetilde{\wp}_i \widetilde{\wp}_{jk} = \widetilde{\wp}_{jk} \widetilde{\wp}_i = 0$.

$$\widetilde{\wp}_j \widetilde{\wp}_i f(\mathbf{x}) = \widetilde{\wp}_j \left[\prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\left(x_i, \mathbf{b}_I^i, \mathbf{a}^I\right) - \tilde{f}_0 \right]$$

$$= \widetilde{\wp}_j \left[\prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\left(x_i, \mathbf{b}_I^i, \mathbf{a}^I\right) \right] - \widetilde{\wp}_j \widetilde{\wp}_0 f(\mathbf{x})$$

$$= \widetilde{\wp}_j \left[\prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\left(x_i, \mathbf{b}_I^i, \mathbf{a}^I\right) \right]$$

$$= \prod_{s=1, i_s \neq j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_j - a_j}{b_j - a_j} r_l\left(\mathbf{b}_I, \mathbf{a}^I\right) \right] - \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\left(\mathbf{b}_I, \mathbf{a}^I\right)$$

$$= \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[r_l\left(\mathbf{b}_I, \mathbf{a}^I\right) - r_l\left(\mathbf{b}_I, \mathbf{a}^I\right)\right] = 0. \tag{A.23}$$

Thus, we have

$$\widetilde{\wp}_j \widetilde{\wp}_i = 0. \tag{A.24}$$

As i and j are symmetric in the formula, we also have

$$\widetilde{\wp}_i \widetilde{\wp}_j = 0, \tag{A.25}$$

i.e.,

$$\widetilde{\wp}_j \widetilde{\wp}_i = \widetilde{\wp}_i \widetilde{\wp}_j = 0. \tag{A.26}$$

$$\widetilde{\wp}_i \widetilde{\wp}_{ij} f(\mathbf{x}) = \widetilde{\wp}_i \left[\prod_{s=1, i_s \neq i, j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\left(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\right) - \tilde{f}_i - \tilde{f}_j - \tilde{f}_0 \right]$$

$$
\begin{aligned}
&= \widetilde{\wp}_i \left[\prod_{s=1, i_s \neq i, j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) \right] \\
&\quad - \widetilde{\wp}_i \widetilde{\wp}_i f(\mathbf{x}) - \widetilde{\wp}_i \widetilde{\wp}_j f(\mathbf{x}) - \widetilde{\wp}_i \widetilde{\wp}_0 f(\mathbf{x}) \\
&= \widetilde{\wp}_i \left[\prod_{s=1, i_s \neq i, j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) \right] - \widetilde{\wp}_i f(\mathbf{x}) \\
&= \prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) - \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&\quad - \prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) + \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) = 0.
\end{aligned} \tag{A.27}
$$

Combining equation (A.19) we have

$$
\widetilde{\wp}_i \widetilde{\wp}_{ij} = \widetilde{\wp}_{ij} \widetilde{\wp}_i = 0. \tag{A.28}
$$

$$
\begin{aligned}
\widetilde{\wp}_i \widetilde{\wp}_{jk} f(\mathbf{x}) &= \widetilde{\wp}_i \left[\prod_{s=1, i_s \neq j, k}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_j, x_k, \mathbf{b}_I^{jk}, \mathbf{a}^I\big) - \tilde{f}_j - \tilde{f}_k - \tilde{f}_0 \right] \\
&= \widetilde{\wp}_i \left[\prod_{s=1, i_s \neq j, k}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_j, x_k, \mathbf{b}_I^{jk}, \mathbf{a}^I\big) \right] \\
&\quad - \widetilde{\wp}_i \widetilde{\wp}_j f(\mathbf{x}) - \widetilde{\wp}_i \widetilde{\wp}_k f(\mathbf{x}) - \widetilde{\wp}_i \widetilde{\wp}_0 f(\mathbf{x}) \\
&= \widetilde{\wp}_i \left[\prod_{s=1, i_s \neq j, k}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_j, x_k, \mathbf{b}_I^{jk}, \mathbf{a}^I\big) \right] \\
&= \prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_i - a_i}{b_i - a_i} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] - \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&= \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \big[r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \big] = 0.
\end{aligned} \tag{A.29}
$$

$$
\begin{aligned}
\widetilde{\wp}_{jk} \widetilde{\wp}_i\ f(\mathbf{x}) &= \widetilde{\wp}_{jk} \left[\prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) - \tilde{f}_0 \right] \\
&= \widetilde{\wp}_{jk} \left[\prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \right] - \widetilde{\wp}_{jk} \widetilde{\wp}_0 f(\mathbf{x}) \\
&= \widetilde{\wp}_{jk} \left[\prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \right]
\end{aligned}
$$

$$
\begin{aligned}
&= \prod_{s=1, i_s \neq j,k}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{(x_j - a_j)(x_k - a_k)}{(b_j - a_j)(b_k - a_k)} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] \\
&\quad - \prod_{s=1, i_s \neq j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_j - a_j}{b_j - a_j} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] \\
&\quad - \prod_{s=1, i_s \neq k}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_k - a_k}{b_k - a_k} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] + \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&= \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \big[r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) + r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \big] = 0.
\end{aligned} \tag{A.30}
$$

Then we have

$$
\widetilde{\wp}_i \widetilde{\wp}_{jk} = \widetilde{\wp}_{jk} \widetilde{\wp}_i = 0. \tag{A.31}
$$

3. $\widetilde{\wp}_{ij}$

We only need to prove that $\widetilde{\wp}_{ik}\widetilde{\wp}_{ij} = \widetilde{\wp}_{kl}\widetilde{\wp}_{ij} = 0$.

$$
\begin{aligned}
\widetilde{\wp}_{ik}\widetilde{\wp}_{ij} f(\mathbf{x}) &= \widetilde{\wp}_{ik} \left[\prod_{s=1, i_s \neq i,j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) - \tilde{f}_i - \tilde{f}_j - \tilde{f}_0 \right] \\
&= \widetilde{\wp}_{ik} \left[\prod_{s=1, i_s \neq i,j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) \right] \\
&\quad - \widetilde{\wp}_{ik}\widetilde{\wp}_i f(\mathbf{x}) - \widetilde{\wp}_{ik}\widetilde{\wp}_j f(\mathbf{x}) - \widetilde{\wp}_{ik}\widetilde{\wp}_0 f(\mathbf{x}) \\
&= \widetilde{\wp}_{ik} \left[\prod_{s=1, i_s \neq i,j}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) \right] \\
&= \prod_{s=1, i_s \neq i,k}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_k - a_k}{b_k - a_k} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \right] \\
&\quad - \prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \\
&\quad - \prod_{s=1, i_s \neq k}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \left[\frac{x_k - a_k}{b_k - a_k} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \right] + \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&= \prod_{s=1, i_s \neq i}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \big[r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) - r_l\big(x_i, \mathbf{b}_I^{i}, \mathbf{a}^I\big) \big] \\
&\quad - \prod_{s=1}^{m} \frac{x_{i_s} - a_{i_s}}{b_{i_s} - a_{i_s}} \big[r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \big] = 0.
\end{aligned} \tag{A.32}
$$

Similarly, we have

$$\widetilde{\wp}_{ij}\widetilde{\wp}_{ik} f(\mathbf{x}) = 0. \tag{A.33}$$

Then

$$\widetilde{\wp}_{ij}\widetilde{\wp}_{ik} = \widetilde{\wp}_{ik}\widetilde{\wp}_{ij} = 0. \tag{A.34}$$

$$\begin{aligned}
\widetilde{\wp}_{kl}\widetilde{\wp}_{ij} f(\mathbf{x}) &= \widetilde{\wp}_{kl}\left[\prod_{s=1, i_s\neq i,j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big) - \tilde{f}_i - \tilde{f}_j - \tilde{f}_0\right] \\
&= \widetilde{\wp}_{kl}\left[\prod_{s=1, i_s\neq i,j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big)\right] \\
&\quad - \widetilde{\wp}_{kl}\widetilde{\wp}_i f(\mathbf{x}) - \widetilde{\wp}_{kl}\widetilde{\wp}_j f(\mathbf{x}) - \widetilde{\wp}_{kl}\widetilde{\wp}_0 f(\mathbf{x}) \\
&= \widetilde{\wp}_{kl}\left[\prod_{s=1, i_s\neq i,j}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\big)\right] \\
&= \prod_{s=1, i_s\neq k,l}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}\left[\frac{(x_k-a_k)(x_l-a_l)}{(b_k-a_k)(b_l-a_l)} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\right] \\
&\quad - \prod_{s=1, i_s\neq k}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}\left[\frac{x_k-a_k}{b_k-a_k} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\right] \\
&\quad - \prod_{s=1, i_s\neq l}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}\left[\frac{x_l-a_l}{b_l-a_l} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\right] + \prod_{s=1}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&= \prod_{s=1}^{m} \frac{x_{i_s}-a_{i_s}}{b_{i_s}-a_{i_s}}\big[r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) + r_l\big(\mathbf{b}_I, \mathbf{a}^I\big)\big] = 0.
\end{aligned} \tag{A.35}$$

Similarly, we have

$$\widetilde{\wp}_{ij}\widetilde{\wp}_{kl} f(\mathbf{x}) = 0. \tag{A.36}$$

Then

$$\widetilde{\wp}_{ij}\widetilde{\wp}_{kl} = \widetilde{\wp}_{kl}\widetilde{\wp}_{ij} = 0. \tag{A.37}$$

The proofs above show that all the projectors $\{\widetilde{\wp}\}$ within each I are mutually orthogonal.

A.2.2. Orthogonality between $\{\widetilde{\wp}\}$ in different I

Suppose we have two subsets I and J of $\{1, 2, \ldots, n\}$ for a given m such that $I \neq J$, and two sets of new projectors $\{\widetilde{\wp}\}$ and $\{\check{\wp}\}$ are defined on I and J, respectively. As at least one variable $x_{i_s} \in I$, say x_s, does not belong to J, then $x_s = a_s$ in $\check{\wp}_t[\widetilde{\wp}_s f(\mathbf{x})]$, which make it vanish because the condition given at the beginning of the appendix is satisfied. Thus,

$$\check{\wp}_t\big[\widetilde{\wp}_s f(\mathbf{x})\big] = 0. \tag{A.38}$$

Similarly,

$$\widetilde{\wp}_s\big[\check{\wp}_t f(\mathbf{x})\big] = 0. \tag{A.39}$$

Then we have

$$\check{\wp}_t\widetilde{\wp}_s = \widetilde{\wp}_s\check{\wp}_t = 0. \tag{A.40}$$

This shows that all of the projectors $\{\widetilde{\wp}\}$ for a given m but in different I are mutually orthogonal.

A.2.3. Orthogonality between $\{\widetilde{\wp}\}$ *and* $\{\wp\}$

As projectors $\{\wp\}$ of the lth order Cut-HDMR have an order equal to or less than l, and $\{\widetilde{\wp}\}$ has $m = l + 1$, then

$$\wp_r\widetilde{\wp}_s f(\mathbf{x}) = 0 \tag{A.41}$$

because some $x_{i_s} = a_{i_s}$ $(i_s \in I)$ which satisfies the condition given at the beginning of the appendix.

Moreover, we also have

$$\widetilde{\wp}_s\wp_r f(\mathbf{x}) = 0 \tag{A.42}$$

because each term of $\wp_r f(\mathbf{x})$ is a function of l or less input variables. Its lth order Cut-HDMR expansion is exact and the corresponding residual is zero. Thus, $\widetilde{\wp}_s\wp_r f(\mathbf{x}) = 0$. Then we have

$$\wp_r\widetilde{\wp}_s = \widetilde{\wp}_s\wp_r = 0. \tag{A.43}$$

Thus, all projectors $\{\widetilde{\wp}\}$ for a given m and all projectors $\{\wp\}$ of the lth order Cut-HDMR are mutually orthogonal.

A.3. Invariance property

We will prove that $f(x_{i_1}, x_{i_2}, \dots, x_{i_s}, \mathbf{a}^{i_1 i_2 \dots i_s})$ $(s = 1, 2, \dots, l)$, $f(x_i, \mathbf{b}_I^i, \mathbf{a}^I)$ and $f(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I)$ $(i, j \in I)$ are invariant to the maximal projector $\mathcal{M}$ in equation (43). Notice that

$$\begin{aligned} f(\mathbf{x}) - r_l(\mathbf{x}) = f_0 + \sum_{i=1}^n f_i + \sum_{1\leqslant i<j\leqslant n} f_{ij} + \cdots \\ + \sum_{1\leqslant i_1<\cdots<i_l\leqslant n} f_{i_1 i_2 \dots i_l}. \end{aligned} \tag{A.44}$$

Then equation (43) can be rewritten as

$$
\begin{aligned}
\mathcal{M}f(\mathbf{x}) &= f(\mathbf{x}) - r_l(\mathbf{x}) + \sum_I \Bigg[\tilde{f}_0 + \sum_{s=1}^{m} \tilde{f}_{i_s} + \sum_{1 \leqslant r < s \leqslant m} \tilde{f}_{i_r i_s} \Bigg] \\
&= f(\mathbf{x}) - r_l(\mathbf{x}) + \sum_I \Bigg[\prod_{t=1}^{m} \frac{x_{i_t} - a_{i_t}}{b_{i_t} - a_{i_t}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&\quad + \sum_{s=1}^{m} \Bigg(\prod_{t=1, i_t \neq i_s}^{m} \frac{x_{i_t} - a_{i_t}}{b_{i_t} - a_{i_t}} r_l\big(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I\big) - \prod_{t=1}^{m} \frac{x_{i_t} - a_{i_t}}{b_{i_t} - a_{i_t}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \Bigg) \\
&\quad + \sum_{1 \leqslant r < s \leqslant m} \Bigg(\prod_{t=1, i_t \neq i_r, i_s}^{m} \frac{x_{i_t} - a_{i_t}}{b_{i_t} - a_{i_t}} r_l\big(x_{i_r}, x_{i_s}, \mathbf{b}_I^{i_r i_s}, \mathbf{a}^I\big) \\
&\quad - \prod_{t=1, i_t \neq i_r}^{m} \frac{x_{i_t} - a_{i_t}}{b_{i_t} - a_{i_t}} r_l\big(x_{i_r}, \mathbf{b}_I^{i_r}, \mathbf{a}^I\big) - \prod_{s=1, i_t \neq i_s}^{m} \frac{x_{i_t} - a_{i_t}}{b_{i_t} - a_{i_t}} r_l\big(x_{i_s}, \mathbf{b}_I^{i_s}, \mathbf{a}^I\big) \\
&\quad + \prod_{t=1}^{m} \frac{x_{i_t} - a_{i_t}}{b_{i_t} - a_{i_t}} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \Bigg) \Bigg]. \qquad \text{(A.45)}
\end{aligned}
$$

The determination of the quantities $\mathcal{M}\, f(x_{i_1}, x_{i_2}, \ldots, x_{i_s}, \mathbf{a}^{i_1 i_2 \ldots i_s})$, $\mathcal{M}\, f(x_i, \mathbf{b}_I^i, \mathbf{a}^I)$ and $\mathcal{M}\, f(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I)$ is achieved by simply substituting the corresponding coordinates $\{x_{i_1}, x_{i_2}, \ldots, x_{i_s}, \mathbf{a}^{i_1 i_2 \ldots i_s}\}$, $\{x_i, \mathbf{b}_I^i, \mathbf{a}^I\}$ and $\{x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I\}$ into equation (A.45).

1. $f(x_{i_1}, x_{i_2}, \ldots, x_{i_s}, \mathbf{a}^{i_1 i_2 \ldots i_s})$

Considering the condition mentioned at the beginning of the appendix, we have

$$
\begin{aligned}
&\mathcal{M}f\big(x_{i_1}, x_{i_2}, \ldots, x_{i_s}, \mathbf{a}^{i_1 i_2 \ldots i_s}\big) \\
&\quad = f\big(x_{i_1}, x_{i_2}, \ldots, x_{i_s}, \mathbf{a}^{i_1 i_2 \ldots i_s}\big) - 0 + \sum_I \Bigg(0 + \sum_{s=1}^{m} 0 + \sum_{1 \leqslant r < s \leqslant m} 0 \Bigg) \\
&\quad = f\big(x_{i_1}, x_{i_2}, \ldots, x_{i_s}, \mathbf{a}^{i_1 i_2 \ldots i_s}\big). \qquad \text{(A.46)}
\end{aligned}
$$

2. $f(x_i, \mathbf{b}_I^i, \mathbf{a}^I)$

Notice that all $\check{\wp}_t f(x_i, \mathbf{b}_I^i, \mathbf{a}^I) = 0$ where $\check{\wp}_t$ belong to J $(J \neq I)$. This is valid because the condition given at the beginning of the appendix is satisfied. Then for $f(x_i, \mathbf{b}_I^i, \mathbf{a}^I)$, equation (A.45) becomes

$$
\begin{aligned}
\mathcal{M}f\big(x_i, \mathbf{b}_I^i, \mathbf{a}^I\big) &= f\big(x_i, \mathbf{b}_I^i, \mathbf{a}^I\big) - r_l\big(x_i, \mathbf{b}_I^i, \mathbf{a}^I\big) + \frac{x_i - a_i}{b_i - a_i} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&\quad + r_l\big(x_i, \mathbf{b}_I^i, \mathbf{a}^I\big) - \frac{x_i - a_i}{b_i - a_i} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \\
&\quad + \sum_{s=1, i_s \neq i}^{m} \Bigg[\frac{x_i - a_i}{b_i - a_i} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) - \frac{x_i - a_i}{b_i - a_i} r_l\big(\mathbf{b}_I, \mathbf{a}^I\big) \Bigg]
\end{aligned}
$$

$$+\sum_{s=1,i_s\neq i}^{m}\Big[r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big)-r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big)$$

$$-\frac{x_i-a_i}{b_i-a_i}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)+\frac{x_i-a_i}{b_i-a_i}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\Big]$$

$$+\sum_{1\leqslant r<s\leqslant m,i_r,i_s\neq i}\Big[\frac{x_i-a_i}{b_i-a_i}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)-\frac{x_i-a_i}{b_i-a_i}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)$$

$$-\frac{x_i-a_i}{b_i-a_i}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)+\frac{x_i-a_i}{b_i-a_i}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\Big]$$

$$=f\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big). \tag{A.47}$$

3. $f(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I)$

Similarly to the treatment above, we have

$$\mathcal{M}f(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I)$$

$$=f\big(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I\big)-r_l\big(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I\big)$$

$$+\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)+\frac{x_j-a_j}{b_j-a_j}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}\big)$$

$$-\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)+\frac{x_i-a_i}{b_i-a_i}r_l\big(x_j,\mathbf{b}_I^j,\mathbf{a}^I\big)$$

$$-\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)$$

$$+\sum_{s=1,i_s\neq i,j}^{m}\Big[\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)-\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\Big]$$

$$+\Big[r_l\big(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I\big)-\frac{x_j-a_j}{b_j-a_j}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big)$$

$$-\frac{x_i-a_i}{b_i-a_i}r_l\big(x_j,\mathbf{b}_I^j,\mathbf{a}^I\big)+\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\Big]$$

$$+\sum_{s=1,i_s\neq i,j}^{m}\Big[\frac{x_j-a_j}{b_j-a_j}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big)-\frac{x_j-a_j}{b_j-a_j}r_l\big(x_i,\mathbf{b}_I^i,\mathbf{a}^I\big)$$

$$-\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)+\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\Big]$$

$$+\sum_{s=1,i_s\neq i,j}^{m}\Big[\frac{x_i-a_i}{b_i-a_i}r_l\big(x_j,\mathbf{b}_I^j,\mathbf{a}^I\big)-\frac{x_i-a_i}{b_i-a_i}r_l\big(x_j,\mathbf{b}_I^j,\mathbf{a}^I\big)$$

$$-\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)+\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\Big]$$

$$
\begin{aligned}
&+\sum_{1\leqslant r<s\leqslant m, i_r, i_s\neq i,j}\left[\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)-\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\right.\\
&\left.-\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)+\frac{(x_i-a_i)(x_j-a_j)}{(b_i-a_i)(b_j-a_j)}r_l\big(\mathbf{b}_I,\mathbf{a}^I\big)\right]\\
&=f\big(x_i,x_j,\mathbf{b}_I^{ij},\mathbf{a}^I\big). \qquad \text{(A.48)}
\end{aligned}
$$

The analysis above proves that $f(x_{i_1}, x_{i_2}, \ldots, x_{i_s}, \mathbf{a}^{i_1 i_2 \ldots i_s})$ $(s = 1, 2, \ldots, l)$, $f(x_i, \mathbf{b}_I^i, \mathbf{a}^I)$ and $f(x_i, x_j, \mathbf{b}_I^{ij}, \mathbf{a}^I)$ $(i, j \in I)$ are invariant to the maximal projector $\mathcal{M}$ in equation (43).

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References

[1] H. Rabitz, O.F. Alis, J. Shorter and K. Shim, Efficient input–output model representations, Comput. Phys. Commun. 115 (1998) 1–10.

[2] O.F. Alis and H. Rabitz, General foundations of high dimensional model representations, J. Math. Chem. 25 (1999) 197–233.

[3] K. Shim and H. Rabitz, Independent and correlated composition behavior of material properties: Application to energy band gaps for the $\mathrm{Ga}_\alpha\mathrm{In}_{1-\alpha}\mathrm{P}_\beta\mathrm{As}_{1-\beta}$ and $\mathrm{Ga}_\alpha\mathrm{In}_{1-\alpha}\mathrm{P}_\beta\mathrm{Sb}_\gamma\mathrm{As}_{1-\beta-\gamma}$ alloys, Phys. Rev. B 58 (1998) 1940–1946.

[4] J. Shorter and H. Rabitz, An efficient chemical kinetics solver using high dimensional model representations, J. Phys. Chem. A 103(36) (1999) 7192–7198.

[5] R.G. Ghanem and P.D. Spanos, *Stochastic Finite Elements: A Spectral Approach* (Springer-Verlag, New York, 1991).

[6] O.F. Alis and H. Rabitz, Efficient implementation of high dimensional model representations, in: *Mathematical and Statistical Methods for Sensitivity Analysis*, ed. A. Saltelli (Wiley, 2000).

[7] S.W. Wang, H. Levy II, G. Li and H. Rabitz, Fully equivalent operational models for atmospheric chemical kinetics within global chemistry-transport models, J. Geophys. Res. 104(D23) (1999) 30,417–30,426.

[8] A. Faliks, R.A. Yetter, C.A. Floudas, S.L. Bernasek, M. Fransson and H. Rabitz, Optimal control of catalytic methanol conversion to formaldehyde, J. Catal. (in press).

[9] W.J. Gordon, Distributive lattices and the approximation of multivariate functions, in: *Proc. Symp. Approximation with Special Emphasis on Spline Functions*, ed. I.J. Schoenberg (Academic Press, New York, 1969) pp. 223–277.