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General foundations of high-dimensional model representations

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A family of multivariate representations is introduced to capture the input–output relationships of high-dimensional physical systems with many input variables. A systematic mapping procedure between the inputs and outputs is prescribed to reveal the hierarchy of correlations amongst the input variables. It is argued that for most well-defined physical systems, only relatively low-order correlations of the input variables are expected to have an impact upon the output. The high-dimensional model representations (HDMR) utilize this property to present an exact hierarchical representation of the physical system. At each new level of HDMR, higher-order correlated effects of the input variables are introduced. Tests on several systems indicate that the few lowest-order terms are often sufficient to represent the model in equivalent form to good accuracy. The input variables may be either finite-dimensional (i.e., a vector of parameters chosen from the Euclidean space R^n) or may be infinite-dimensional as in the function space $C^n[0, 1]$. Each hierarchical level of HDMR is obtained by applying a suitable projection operator to the output function and each of these levels are orthogonal to each other with respect to an appropriately defined inner product. A family of HDMRs may be generated with each having distinct character by the use of different choices of projection operators. Two types of HDMRs are illustrated in the paper: ANOVA-HDMR is the same as the analysis of variance (ANOVA) decomposition used in statistics. Another cut-HDMR will be shown to be computationally more efficient than the ANOVA decomposition. Application of the HDMR tools can dramatically reduce the computational effort needed in representing the input–output relationships of a physical system. In addition, the hierarchy of identified correlation functions can provide valuable insight into the model structure. The notion of a model in the paper also encompasses input–output relationships developed with laboratory experiments, and the HDMR concepts are equally applicable in this domain. HDMRs can be classified as non-regressive, non-parametric learning networks. Selected applications of the HDMR concept are presented along with a discussion of its general utility.

1. Introduction

The physical models of various phenomena and their resultant mathematical structure often contain many input variables. Such models act to represent real world or laboratory processes, and this paper will generally use the word “model” to also en-

compass working directly with the laboratory variables and observations. In some cases the system variables serve as controls to be set in the laboratory and in other circumstances they are internal model variables whose values may be uncertain. In either case, a general desire is to deduce the detailed structure of the n-dimensional variable space in order to identify regions of special impact on the model or observed output. Without any *a priori* physical assumption on the nature of the model input–output relationships, construction of a full space analysis would be NP-complete with computational complexity scaling exponentially as $\sim s^n$, where s is the number of sample values for each input variable. This problem is sometimes referred to as the *curse of dimensionality*, i.e., without any regularization or other form of simplification, learning the multivariate input–output function from its sample values is computationally or observationally NP-complete in the dimension of its input variables. Stone [32] showed that, using local polynomial regression, one can achieve a rate of convergence $\varepsilon_N = N^{-p/(2p+n)}$ with N being the number of sample points and p being the degree of the smoothness of the function, e.g., $p = 2$ implies that the function is twice differentiable. It is easy to see how the curse of dimensionality appears. Without a high degree of smoothness ($p \ll n$), $\varepsilon_N = N^{-p/n}$, and one needs $\sim s^{n/p}$ sample points to approximate the function to a resolution of $1/s$. So, without any *a priori* knowledge of the output, the approximation/interpolation problem appears to be NP-complete. The high-dimensional model representations (HDMR) introduced in this paper aim to show that a dramatic reduction in this scaling is often expected to arise in well-defined physical systems due to the presence of only low-order correlations amongst the input variables having a significant impact upon the output.

The model output will be a *function* if the input variables are chosen from a Euclidean space R^n and a *functional* if the input variables come from an infinite-dimensional function space like $C[0, 1]$ (i.e., the space of continuous functions on the unit interval). The HDMR expansions introduced here are especially useful for the purpose of representing the outputs of a physical system when the number of input variables is large. The HDMR expansions are based on exploiting the correlated effects of the input variables, which are naturally created by the input–output mapping. The term "correlation" employed here is generally distinct from that employed in statistics, as the input variables often will not be random. We assume that the model output(s) is rationally behaved in terms of the input variables (i.e., the output is a well-defined function(al), but rapid or even discontinuous behavior would still be permitted). The high dimensionality of the input space and the expense of performing model calculations or experiments often prevent a full sampling of the input space (i.e., $\sim s^n$ computer simulations or experiments). The notion of "high" dimensionality is system-dependent, with some situations being considered high for practical reasons at $n \sim$ 3–5, while others will only reach that level of complexity for $n \gg 10$ or more.

With the comments above as background we seek a fast algorithm which can circumvent the apparent exponential difficulty of the high-dimensional mapping problem. In the case of function mapping the HDMR expansions can be written in the

following form, for $f(x) \equiv f(x_1, x_2, \ldots, x_n)$ representing the mapping between the input variables $x_1, x_2, \ldots, x_n$ defined on the domain $\Omega \subset R^n$ and the output f:

$$f(x) \equiv f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j) + \cdots + f_{12\ldots n}(x_1, x_2, \ldots, x_n). \qquad (1)$$

An analogous expansion applies to functional mapping. Here f_0 denotes the zeroth-order effect which is a constant everywhere in the domain Ω. The function $f_i(x_i)$ gives the effect associated with the variable x_i acting independently, although generally nonlinearly, upon the output f. The function $f_{ij}(x_i, x_j)$ describes the cooperative effects of the variables x_i and x_j, and higher-order terms reflect the cooperative effects of increasing numbers of variables acting together to impact upon f. The last term $f_{12\ldots n}(x_1, \ldots, x_n)$ gives any residual dependence of all the variables locked together in a cooperative way to influence the output f. If there is no cooperation between the input variables, then only zeroth-order and first-order terms will appear in the expansion. However, even to first order the expansion is not a linear superposition, as $f_i(x_i)$ could have an arbitrary dependence on x_i. The notion of 0th, 1st, 2nd order, etc. in the HDMR expansion should not be confused with the terminology of a Taylor series; the HDMR expansion is exact and always of finite order. The HDMR expansion is a very efficient formulation of the physical output if higher-order variable correlations are weak, permitting the physical model to be captured by the first few lower-order terms. The resultant computational or experimental effort to determine the expansion functions will scale polynomically with n rather than the traditional view of it being exponential with n. The choice of input variables can be important, but evidence suggests that often no special effort is required to find rapid convergence of the HDMR expansion *for most well-defined physical systems*. Typically, physical input variables are chosen, often with much insight or experience, to have distinct roles, which aids in the convergence of the HDMR. In some cases suitable transformations of the variables may be helpful to simplify the analysis.

The HDMR has a structure analogous to the many-body expansions used in molecular physics [23] to represent potential surfaces created by a system of atoms. Generally, two-body terms dominate and rarely are terms beyond third-order significant. The many-body expansions can be viewed as a special case of an HDMR which rapidly converges for particular physical reasons. Similar rapidly convergent cluster expansions are utilized in statistical mechanics [10]. Expansions of the form of equation (1) have been introduced before for various additional purposes [5,9,24,30], but they have not been extensively exploited. The HDMR concept rests on suggesting that a similar rapid loss of correlation exists under more general physical conditions. Perhaps the best evidence for this conjecture lies in statistics where rarely do more than input covariances play a significant role. The latter behavior can depend on the dynamic range of the input variables, but the observed lack of higher-order correlations appears to be generic. Conversely, an HDMR may not be of practical utility (i.e., high-order terms play a role) for arbitrary mathematical functions, although equation (1) is always an exact representation.

In order to understand the effects of each of the terms in the HDMR expansion, projection operators $P_{i_1 i_2 \ldots i_l}$ may be introduced so that $P_{i_1 i_2 \ldots i_l} f = f_{i_1 i_2 \ldots i_l}$ determines a particular term in the HDMR expansion. The orthogonality of the projection operators ensures that the terms within and between each order give unique correlated information about the variables contributing to the output function $f(x)$. The sum of the full set of projection operators $\{P_{i_1 i_2 \ldots i_l}\}$ provides a resolution of the identity operator and different sets of projection operators give rise to distinct HDMR expansions. The choice of a particular HDMR expansion depends on the application and the nature of any constraints for sampling the input variables $x_1, \ldots, x_n$. The input space is assumed to be a normed vector space furnished with an inner product expressed in terms of a suitable measure.

Attempts at approximating multivariate functions by linear or nonlinear superpositions of functions have a long history, and some relevant cases are mentioned here as further background. *Projection pursuit* algorithms [3,7,13,33] approximate the multivariate function $f(x)$ in the form

$$f(x) \equiv f(x_1, x_2, \ldots, x_n) = \mu + \sum_{i=1}^{K} f_i \left(\sum_{k=1}^{n} \beta_{ik} x_k \right), \tag{2}$$

where $\vec{\beta}_i \equiv [\beta_{i1}, \ldots, \beta_{in}]$ represent the projection directions and μ is taken to be the average of the function. The parameter vectors $\vec{\beta}_i$ and functions f_i are estimated from the data. One may view (2) as a special case of (1) using linear combinations of the original variables and truncating the expansion to the first order. *Multilayer perceptrons* (MLPs) [17] used in artificial neural networks approximate the multivariate function $f(x)$ in the following form:

$$f(x) = h \left(\sum_{i=1}^{K} \alpha_i g \left(\sum_{k=1}^{n} \beta_{ik} x_k \right) \right), \tag{3}$$

where h and g are arbitrary nonlinear functions (i.e., this is an MLP with a single *hidden layer*). Such a *learning network* is trained with a given set of input and output values and an MLP approximation seeks to find the scalars α_k and the vectors $\vec{\beta}_i$ by least squares minimization. *Radial basis functions* [18] have been used to approximate $f(x)$ as a nonlinear function of its input variables under a regularization criteria. This approach under certain conditions [18] leads to the expansion

$$f(x) = \sum_{i=1}^{K} \beta_i f_i\big(\|x - u_i\|\big) + \mathcal{P}(x), \tag{4}$$

where the u_i are centers similar to the knots of splines, the β_i are constants, the f_k are a chosen set of *radial basis functions* (e.g., a Gaussian) and $\mathcal{P}$ is a polynomial. The coefficients are then fitted to data using least-squares minimization. Although the representations above are useful for particular applications, there is no general rule of thumb to choose one over another. There are not widely accepted procedures for

determining the number of hidden layers, number of functions, etc. The parameters of the networks are obtained by least-squares minimization and typically the objective functional is not globally convex and has many local minima, which may result in a nonunique representation.

The above representations are often quoted as inspired by a theorem of Kolmogorov [15] which states that a multivariate function defined on the unit cube $K^n = [0,1]^n$ can be represented in the following way:

$$f(x_1, x_2, \ldots, x_n) = \sum_{q=1}^{2n+1} g\big(\lambda_1 \phi_q(x_1) + \cdots + \lambda_n \phi_q(x_n)\big), \tag{5}$$

i.e., any multivariate function can be written as a linear superposition of univariate functions. Although the functions ϕ_q are continuous, they are highly nonsmooth and their practical utility for approximation/interpolation appears very limited [8]. The HDMR technique aims to represent multivariate functions arising in physical contexts rather than for arbitrary function interpolation. As argued earlier, in most well-defined physical systems it is natural to expect very low-order correlations amongst the input variables for their action upon the output function $f(x)$. There is a predisposition towards this behavior in describing physical systems as one naturally chooses the variables to act as independently as possible. In light of the theorem of Kolmogorov, it appears that although the natural variables in typical physical systems are not perfect in the sense of equation (5), the additional low-order correlations are easily managed.

There is no unique decomposition of the model output $f(x_1, x_2, \ldots, x_n)$ in the form of equation (1). This richness of the HDMR expansions may be exploited for a specific representation objective. For example, in the case of uncertainty analysis of the model output (e.g., an analysis of the variance of the output), one should choose the component functions in the HMDR so that they represent the independent contributions of input variables to the overall uncertainty of the output. Such an ANOVA-HDMR used in statistics can measure the importance of the input variable variance upon the variance of the output. In this case each component function is a random quantity uniquely contributing to the overall variance of the output. The hierarchical formulation of ANOVA-HDMR allows for the identification of how each input variable or group of input variables determines the variance of the output. In this way, ANOVA-HDMR also supplies a nonlinear sensitivity analysis of the model output. A drawback of the traditional ANOVA-HDMR is the need for Monte Carlo simulations to compute the component functions [12,22]. Cut-HDMR is a different HDMR expansion using a specific sampling of the model output to generally provide a computationally more efficient representation than ANOVA-HDMR. If an uncertainty analysis of the model output is of interest, then a cut-HDMR can be easily converted into ANOVA-HDMR of the output. This approach is generally computationally more efficient than the direct route of computing the ANOVA-HDMR of the model output, and this point is discussed in the paper.

The paper is organized as follows. Section 2 gives the general formulation of the HDMR function expansion in terms of projection operators where the input variables reside in R^n. Sections 2.1 and 2.2 presents two particular HDMR function expansions. Section 3 considers the HDMR expansion for functionals where the input values come from the n-fold product space X^n, where X is an arbitrary linear topological function space. The appendix gives a primer on functional integrals essential to the understanding of the material presented in section 3. The numerical examples in the paper are chosen to illustrate the capabilities of the HDMR concept. No detailed exposition is given in the physical background of the examples, as a full elaboration appears elsewhere as cited. In this regard, the present paper aims to present the general foundations of HDMR which are not set forth in the works illustrating the concepts. Section 4 presents a general discussion about further potential applications of the HDMR tools. Concluding remarks and future perspectives are given in section 5.

2. Function HDMR

We assume that the input–output relationship of a physical model is represented by a real, scalar function $f(x) \equiv f(x_1, x_2, \ldots, x_n)$ defined on the unit cube $K^n = \{(x_1, x_2, \ldots, x_n)\colon\ 0 \leqslant x_i \leqslant 1,\ i = 1, 2, \ldots, n\}$. The extension to an output vector is readily apparent as each vector (function) component can be treated separately. $f(x)$ belongs to a linear vector space of functions denoted by X. A measure μ on Borel subsets of K^n is defined so that $\{K^n, \mathcal{B}(K^n), \mu)\}$ becomes a measure space (with $\mathcal{B}(K^n)$ denoting the Borel σ-algebra on K^n). We consider the subspace of X to consist of all integrable functions with respect to μ. We further stipulate that μ is a product measure with unit mass and has a density, i.e.,

$$\mathrm{d}\mu(x) \equiv \mathrm{d}\mu(x_1, \ldots, x_n) = \prod_{i=1}^{n} \mathrm{d}\mu_i(x_i), \qquad \int_{K^1} \mathrm{d}\mu_i(x_i) = 1,$$

$$\mathrm{d}\mu(x) = g(x)\,\mathrm{d}x = \prod_{i=1}^{n} g_i(x_i)\,\mathrm{d}x_i, \tag{6}$$

where $g_i(x_i)$ is the marginal density of the input x_i.

The inner product $\langle \cdot, \cdot \rangle$ on X induced by the measure μ is defined as follows:

$$\langle f, h \rangle \equiv \int_{K^n} f(x) h(x)\,\mathrm{d}\mu(x), \qquad f(x), h(x) \in X. \tag{7}$$

Two functions $f(x)$ and $h(x)$ will be called orthogonal if $\langle f, h \rangle = 0$. Note that functions $f(x)$ and $h(x)$ may depend on different sets of components of the input vector x. The norm $\| \cdot \|_X$ on X induced by the above inner product is defined as follows:

$$\left\| f(x) \right\|_X \equiv \left(\langle f, f \rangle \right)^{1/2} \equiv \left(\int_{K^n} f^2(x)\,\mathrm{d}\mu(x) \right)^{1/2}. \tag{8}$$

We now define the following decomposition of X into subspaces whose mutual intersections are empty:

Definition. $\mathcal{V}_0, \{\mathcal{V}_i\}, \{\mathcal{V}_{ij}\}_{i<j}, \ldots, \mathcal{V}_{12\ldots n} \subset X$ are defined as follows:

$$
\begin{aligned}
\mathcal{V}_0 &\equiv \{f \in X\colon\ f = C,\ \text{where } C \in R \text{ is a constant}\},\\
\mathcal{V}_i &\equiv \Bigg\{ f \in X\colon\ f = f_i(x_i) \text{ is a univariate function of the input } x_i\\
&\qquad\qquad \text{with } \int_{K^1} f_i(x_i)\,\mathrm{d}\mu_i(x_i) = 0 \Bigg\},\\
\mathcal{V}_{ij} &\equiv \Bigg\{ f \in X\colon\ f = f_{ij}(x_i, x_j) \text{ is a bivariate function of the inputs } x_i, x_j\\
&\qquad\qquad \text{with } \int_{K^1} f_{ij}(x_i, x_j)\,\mathrm{d}\mu_k(x_k) = 0,\ k = i, j \Bigg\},\\
\mathcal{V}_{i_1\ldots i_l} &\equiv \Bigg\{ f \in X\colon\ f = f_{i_1\ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l}) \text{ is an } l\text{-variate function of the}\\
&\qquad\qquad \text{inputs } x_{i_1}, \ldots, x_{i_l}\\
&\qquad\qquad \text{with } \int_{K^1} f_{i_1\ldots i_l}(x_{i_1}, \ldots, x_{i_l})\,\mathrm{d}\mu_k(x_k) = 0, \quad k = i_1, \ldots, i_l \Bigg\},\\
&\ \ \vdots\\
\mathcal{V}_{12\ldots n} &\equiv \Bigg\{ f \in X\colon\ f = f_{12\ldots n}(x_1, x_2, \ldots, x_n) \text{ is an } n\text{-variate function of all inputs}\\
&\qquad\qquad \text{with } \int_{K^1} f_{12\ldots n}(x_1, x_2, \ldots, x_n)\,\mathrm{d}\mu_k(x_k) = 0,\ k = i_1, \ldots, i_l \Bigg\}. \qquad (9)
\end{aligned}
$$

The integral null property introduced above in any subspace $\mathcal{V}_{i_1 i_2\ldots i_l}$ serves to assure that the functions are orthogonal:

$$\langle f_{i_1\ldots i_s}, f_{j_1\ldots j_p} \rangle = 0 \qquad (10)$$

for at least one index differing in $\{i_1, \ldots, i_s\}$ and $\{j_1, \ldots, j_p\}$, and s may be the same as p.

Lemma 1. The following proposition can be deduced immediately from the definition above: X is the direct sum of the subspaces defined above, i.e.,

$$X = \mathcal{V}_0 \oplus \sum_i \mathcal{V}_i \oplus \sum_{i<j} \mathcal{V}_{ij} \oplus \cdots \oplus \sum_{i_1<i_2<\cdots<i_l} \mathcal{V}_{i_1 i_2\ldots i_l} \oplus \cdots \oplus \mathcal{V}_{12\ldots n}, \qquad (11)$$

where $\oplus$ denotes the direct sum operator. The corollary to this proposition is that $f(x) \in X$ can be written as

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i<j} f_{ij}(x_i, x_j) + \cdots + f_{12\ldots n}(x_1, x_2, \ldots, x_n). \tag{12}$$

Decomposition (11) of X is unique subject to the choice of measure in (6), which in turn implies that expansion (12) is unique.

Proof. We will determine the individual terms in expression (12) constructively and show uniqueness. Uniqueness of decomposition (11) then follows from this result. We first fix some notation. The conditional mean $\mathbf{M}^{i_1 i_2 \ldots i_l} f(x)$ of the output function with respect to the group of input variables $\{x_{i_1}, x_{i_2}, \ldots, x_{i_l}\}$ is denoted as follows:

$$\mathbf{M}^{i_1 i_2 \ldots i_l} f(x) = \int_{K^{n-l}} f(x) \left[\prod_{j \notin \{i_1, \ldots, i_l\}} \mathrm{d}\mu_j(x_j) \right]. \tag{13}$$

The unconditional mean of the function $f(x)$ is given by

$$\mathbf{M} f(x) = \int_{K^n} f(x)\, \mathrm{d}\mu(x). \tag{14}$$

Now we define the functions f_0, $\{f_i(x_i)\}_i$, etc. recursively as follows:

$$\begin{aligned}
f_0 &\equiv \mathbf{M} f(x), \\
f_i(x_i) &\equiv \mathbf{M}^i f(x) - f_0, \\
f_{ij}(x_i, x_j) &\equiv \mathbf{M}^{ij} f(x) - f_i(x_i) - f_j(x_j) - f_0, \\
&\vdots \\
f_{i_1 \ldots i_l}(x_{i_1}, \ldots, x_{i_l}) &\equiv \mathbf{M}^{i_1 \ldots i_l} f(x) - \sum_{j_1 < \cdots < j_{l-1} \subset \{i_1, \ldots, i_l\}} f_{j_1 \ldots j_{l-1}}(x_{j_1}, \ldots, x_{j_{l-1}}) \\
&\quad - \sum_{j_1 < \cdots < j_{l-2} \subset \{i_1, \ldots, i_l\}} f_{j_1 \ldots j_{l-2}}(x_{j_1}, \ldots, x_{j_{l-2}}) - \cdots \\
&\quad - \sum_{j \subset \{i_1, \ldots, i_l\}} f_j(x_j) - f_0, \\
&\vdots \\
f_{12\ldots n}(x) &\equiv f(x) - f_0 - \sum_i f_i(x_i) - \sum_{ij} f_{ij}(x_i, x_j) - \cdots.
\end{aligned} \tag{15}$$

It is evident that $f_0 \in \mathcal{V}_0$, $f_i(x_i) \in \mathcal{V}_i$ and lastly $f_{12\ldots n} \in \mathcal{V}_{12\ldots n}$. □

Lemma 2. (11) suggests the following family of projection operators defined from X into one of the subspaces above:

$$f_0 \equiv P_0 f(x) = \mathbf{M} f(x),$$

$$
\begin{aligned}
f_i(x_i) &\equiv P_i f(x) = \mathbf{M}^i f(x) - P_0 f(x),\\
f_{ij}(x_i, x_j) &\equiv P_{ij} f(x) = \mathbf{M}^{ij} f(x) - P_i f(x) - P_j f(x) - P_0 f(x),\\
&\vdots\\
f_{i_1\ldots i_l}(x_{i_1}, \ldots, x_{i_l}) &\equiv P_{i_1\ldots i_l} f(x) = \mathbf{M}^{i_1\ldots i_l} f(x) - \sum_{j_1<\cdots<j_{l-1}\subset\{i_1,\ldots,i_l\}} P_{j_1\ldots j_{l-1}} f(x)\\
&\quad - \sum_{j_1<\cdots<j_{l-2}\subset\{i_1,\ldots,i_l\}} P_{j_1\ldots j_{l-2}} f(x) - \cdots\\
&\quad - \sum_{j\subset\{i_1,\ldots,i_l\}} P_j f(x) - P_0 f(x). \qquad (16)
\end{aligned}
$$

These operators are chosen so that the variational problem

$$
\min_u \left\| f(x) - u \right\|_X, \quad u \in \mathcal{V}_0 \oplus \sum_i \mathcal{V}_i \oplus \sum_{i<j} \mathcal{V}_{ij} \oplus \cdots \oplus \sum_{i_1<i_2<\cdots<i_l} \mathcal{V}_{i_1\ldots i_l}, \qquad (17)
$$

is minimized with

$$
u = \left(P_0 + \sum_i P_i + \sum_{i<j} P_{ij} + \cdots + \sum_{i_1<i_2<\cdots<i_l} P_{i_1 i_2\ldots i_l} \right) f(x). \qquad (18)
$$

Proof. Proving assertion (18) can be established by finding the extremal value of the functional $\mathcal{J}$ defined below:

$$
\begin{aligned}
\varepsilon_l(x) &\equiv f(x) - u = f(x) - f_0 - \sum_i f_i(x_i) - \sum_{i<j} f_{ij}(x_i, x_j) - \cdots\\
&\quad - \sum_{i_1<\cdots<i_l} f_{i_1\ldots i_l}(x_{i_1}, \ldots, x_{i_l}),\\
\mathcal{J} &\equiv \left\| f(x) - u \right\|_X^2 = \int_{K^n} \left[\varepsilon_l(x) \right]^2 \mathrm{d}\mu(x), \qquad (19)
\end{aligned}
$$

with the constraints $f_0 \in \mathcal{V}_0$, $f_i(x_i) \in \mathcal{V}_i$, etc. $\varepsilon_l(x)$ is the error of approximation at the lth level.

The proof will be by induction. For $l = 0$,

$$
\mathcal{J} = \int_{K^n} \left[f(x) - f_0 \right]^2 \mathrm{d}\mu(x); \qquad (20)
$$

setting the first variation of $\mathcal{J}$ to zero we get first-order necessary conditions for a minimum:

$$
\frac{\delta \mathcal{J}}{\delta f_0} = -2 \int_{K^n} \left[f(x) - f_0 \right] \mathrm{d}\mu(x) = 0 \quad \Rightarrow \quad f_0 = \int_{K^n} f(x)\, \mathrm{d}\mu(x). \qquad (21)
$$

Lagrange multipliers $\lambda_{i_1 i_2\ldots i_l}$ are introduced below to incorporate the constraints in (9) into the the optimization functional $\mathcal{J}$. The augmented functional is $\mathcal{J}'$.

For $l = 1$,

$$\mathcal{J}' = \int_{K^n} \left[f(x') - f_0 - \sum_{i=1}^{n} f_i(x'_i) \right]^2 \mathrm{d}\mu(x') + \sum_{i=1}^{n} \lambda_i \int_{K^1} f_i(x'_i)\, \mathrm{d}\mu_i(x'_i), \quad (22)$$

$$\frac{\partial \mathcal{J}'}{\partial \lambda_i} = \int_{K^1} f_i(x'_i)\, \mathrm{d}\mu_i(x'_i) = 0, \quad i = 1, 2, \ldots, n, \quad (23)$$

$$\frac{\partial \mathcal{J}'}{\partial f_0} = -2 \int_{K^n} \left[f(x') - f_0 - \sum_j f_j(x'_j) \right] \mathrm{d}\mu(x') = 0, \quad (24)$$

$$\frac{\delta \mathcal{J}'}{\delta f_i(x_i)} = -2 \int_{K^n} \left[f(x') - f_0 - \sum_j f_j(x'_j) \right] \delta(x_i - x'_i)\, \mathrm{d}\mu(x') + \lambda_i = 0. \quad (25)$$

Here $\delta(x_i - x'_i)$ is a Dirac delta function. Equations (23) and (24) together imply

$$f_0 = \int_{K^n} f(x)\, \mathrm{d}\mu(x) = \mathbf{M} f(x). \quad (26)$$

Equations (23) and (25) give

$$-2 g_i(x_i) \left[\mathbf{M}^i f(x) + f_0 - f_i(x_i) \right] + \lambda_i. \quad (27)$$

Integrating this last equation with respect to the variable x_i and using the constraint $\int f_i(x_i)\, \mathrm{d}\mu_i(x_i) = 0$ along with (26) gives $\lambda_i = 0$, resulting in the conclusion

$$f_i(x_i) = \mathbf{M}^i f(x) - f_0. \quad (28)$$

Now, assuming that (18) is true for $l - 1$, we minimize the functional

$$\begin{aligned} \mathcal{J}' = \int_{K^n} \Bigg[& f(x') - f_0 - \sum_{i=1}^{n} f_i(x'_i) - \cdots \\ & - \sum_{j_1 < \cdots < j_l} f_{j_1 \ldots j_l}(x'_{j_1}, \ldots, x'_{j_l}) \Bigg]^2 \mathrm{d}\mu(x') \\ & + \sum_{i_1 < \cdots < i_l} \sum_{k \in \{i_1, i_2, \ldots, i_l\}} \lambda^k_{i_1 \ldots i_l} \int_{K^1} f_{i_1 \ldots i_l}(x'_{i_1}, \ldots, x'_{i_l})\, \mathrm{d}\mu_k(x'_k), \end{aligned}$$

$$\frac{\partial \mathcal{J}'}{\partial \lambda^k_{i_1 \ldots i_l}} = \int_{K^1} f_{i_1 \ldots i_l}(x'_k)\, \mathrm{d}\mu_k(x'_k) = 0, \quad k = i_1, i_2, \ldots, i_l, \quad (29)$$

$$\begin{aligned} \frac{\delta \mathcal{J}'}{\delta f_{i_1 \ldots i_l}(x_{i_1}, \ldots, x_{i_l})} = -2 \int_{K^n} \Bigg[& f(x') - f_0 - \sum_{i=1}^{n} f_i(x'_i) - \cdots \\ & - \sum_{j_1 < \cdots < j_l} f_{j_1 \ldots j_l}(x'_{j_1}, \ldots, x'_{j_l}) \Bigg] \delta(x_{i_1} - x'_{i_1}) - \cdots \end{aligned}$$

$$- \delta\big(x_{i_l} - x'_{i_l}\big)\,\mathrm{d}\mu(x') + \sum_{k\in\{i_1,\ldots,i_l\}} \lambda^k_{i_1\ldots i_l} \prod_{\substack{j\in\{i_1,\ldots,i_l\}\\ j\neq k}} \delta\big(x_j - x'_j\big). \tag{30}$$

Equations (29) and (30) together imply

$$-2\left[\int_{K^n} f(x')\,\mathrm{d}\mu^{i_1\ldots i_l}(x') - f_0 - \sum_{k\in\{i_1,\ldots,i_l\}} f_k(x_k) - \cdots - f_{i_1\ldots i_l}(x_{i_1},\ldots,x_{i_l})\right] + \sum_{k\in\{i_1,\ldots,i_l\}} \lambda^k_{i_1\ldots i_l} \prod_{\substack{j\in\{i_1,\ldots,i_l\}\\ j\neq k}} \delta\big(x_j - x'_j\big). \tag{31}$$

Integrating (31) with respect to the variables $x_{i_1}, x_{i_2}, \ldots, x_{i_l}$ and using the identity in equation (29) we get the following equations for the Lagrange multipliers $\lambda^k_{i_1\ldots i_l}$:

$$\begin{bmatrix} 1 & \delta(x_{i_2}-x'_{i_2}) & \cdots & & \delta(x_{i_l}-x'_{i_l}) \\ \delta(x_{i_1}-x'_{i_1}) & 1 & \delta(x_{i_3}-x'_{i_3}) & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \\ & & & 1 & \delta(x_{i_l}-x'_{i_l}) \\ \delta(x_{i_1}-x'_{i_1}) & \cdots & & \delta(x_{i_{l-1}}-x'_{i_{l-1}}) & 1 \end{bmatrix} \times \begin{bmatrix} \lambda^{i_1}_{i_1\ldots i_l} \\ \lambda^{i_2}_{i_1\ldots i_l} \\ \vdots \\ \vdots \\ \lambda^{i_l}_{i_1\ldots i_l} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{bmatrix}.$$

The above equations are satisfied only if the $\lambda^k_{i_1\ldots i_l}$ are identically zero. Equation (31) then gives

$$\begin{aligned} f_{i_1\ldots i_l}(x_{i_1},\ldots,x_{i_l}) &= \int_{K^{n-l}} f(x')\,\mathrm{d}\mu^{i_1 i_2\ldots i_l}(x') - \sum_{j_1<\cdots<j_{l-1}\subset\{i_1,\ldots,i_l\}} f_{j_1\ldots j_{l-1}}(x_{j_1},\ldots,x_{j_{l-1}}) \\ &\quad - \sum_{j_1<\cdots<j_{l-2}\subset\{i_1,\ldots,i_l\}} f_{j_1\ldots j_{l-2}}(x_{j_1},\ldots,x_{j_{l-2}}) - \cdots - \sum_{j\in\{i_1,\ldots,i_l\}} f_j(x_j) - f_0. \end{aligned} \tag{32}$$

Importantly, each of these functions $f_{i_1,\ldots,i_l}$ is determined separately in a sequence starting from the lower members and moving up. □

Returning again to the collection of projection operators, we observe that they have the following properties:

1. Idempotency:

$$P^2_{i_1 i_2 \ldots i_l} \equiv P_{i_1 i_2 \ldots i_l} \neq 0, \quad i_1 < i_2 < \cdots < i_l \subset \{1, 2, \ldots, n\}. \tag{33}$$

2. Orthogonality:

$$P_{i_1 i_2 \ldots i_l} P_{j_1 j_2 \ldots j_k} \equiv \begin{cases} 0, & l \neq k, \\ P_{i_1 i_2 \ldots i_l} \delta_{i_1 j_1} \delta_{i_2 j_2} \cdots \delta_{i_l j_l}, & l = k, \end{cases} \tag{34}$$

   with the symbol δ_{ij} being the Kronecker delta function. In (1) and (2), the composition of projection operators is understood to imply an integration over the input variable space, and the relation $l = k$ or $l \neq k$ refers to comparing all the indices $i_1 i_2 \ldots i_l$ and $j_1 j_2 \ldots j_k$.

3. Resolution of the identity:

$$P_0 + \sum_i P_i + \sum_{i<j} P_{ij} + \cdots + P_{12\ldots n} = \mathbf{1}, \tag{35}$$

   where **1** denotes the identity operator.

Corollary 1. Operators defined by

$$Q_l = P_0 + \sum_i P_i + \sum_{i<j} P_{ij} + \cdots + \sum_{i_1<i_2<\cdots<i_l \subset \{1,2,\ldots,n\}} P_{i_1 i_2 \ldots i_l} \tag{36}$$

are also projectors.

Corollary 2. An important property of the HDMR is that, if a set of output-model functions obey a set of linear-superposition conservation laws (e.g., conservation of mass), then their HDMR expansion to any order also obeys these conservation law(s) order-by-order. Given the output functions $\{f^1(x), f^2(x), \ldots, f^N(x)\}$, suppose that they obey the following m conservation laws:

$$\sum_{j=1}^{N} w_{kj} f^j(x) = c_k, \quad k = 1, 2, \ldots, m, \tag{37}$$

where w_{kj} are constants. Then these conservation laws are obeyed by $Q_l f^j(x)$ for $0 \leqslant l \leqslant N$, i.e.,

$$\sum_{j=1}^{N} w_{kj} Q_l f^j(x) = c_k, \quad k = 1, 2, \ldots, m, \ l = 0, 1, 2, \ldots, N. \tag{38}$$

This result is obtained by using the following identities:

$$\sum_{j=1}^{N} w_{kj} P_{i_1 \ldots i_l} f^j(x) = \begin{cases} 0, & P_{i_1 \ldots i_l} \neq P_0, \\ c_k, & P_{i_1 \ldots i_l} = P_0. \end{cases} \tag{39}$$

Corollary 3. The properties of the projection operators assure the following: (1) The projection of f to form $f_{i_1 i_2 \ldots i_l}$ is unique given the operator $P_{i_1 i_2 \ldots i_l}$. (2) The functions $f_{i_1 i_2 \ldots i_l}$ and $f_{j_1 j_2 \ldots j_k}$ are independent and orthogonal provided that at least one member of $\{i_1 i_2 \ldots i_l\}$ and $\{j_1 j_2 \ldots j_k\}$ differ from each other. (3) The HDMR expansion has a finite number of terms that exactly represent $f(x)$. The demand that $P_{i_1 i_2 \ldots i_l} \neq 0$ assures that each order of correlation in $f(x)$ is allowed to be naturally identified. The HDMR expansion functions f_0, $f_i(x_i)$, $f_{ij}(x_{ij})$, etc. are understood to be particular types of correlation functions in relation to the properties of the projection operators as explained later.

The HDMR expansion may be understood in terms of $\mathbf{1} \cdot f(x) = f(x)$, where **1** is the unit operator. We may represent **1** in many ways, such as in terms of tensor products of orthogonal functions in each of the variables x_i. The latter representations of $f(x)$ are complete, but they contain an infinite number of terms. The key to the HDMR is the choice of **1** as a hierarchy of projections into subspaces of increasing dimensions playing on the natural expectation of rapidly diminishing contributions from the higher spaces corresponding to high-order correlations amongst the input variables. An important property of HDMR expansions is that they will all converge at the same order. If a choice of the measure μ for a function f gives a HDMR that converges at order L with the error O(ε), then another HDMR defined by the measure μ' will also converge at order L with the error O(ε). However, the expansion functions $f_{i_1 \ldots i_l}(\cdot)$, $l \leqslant L$, in each case will be different. In this sense, the correlation interpretation of the function $f_{i_1 \ldots i_l}(\cdot)$ is associated with the measure used to define their corresponding HDMR. The equivalence of one converged HDMR with respect to any other may be exploited to calculate a convenient one and convert it to another more suitable HDMR for a particular application (see figure 1 below).

The HDMR expansion (1) is used in statistics as the ANOVA (analysis of variance) decomposition [5,24] of a multivariate statistical quantity $f(x_1, \ldots, x_n)$ which depends on independently distributed random variables $x_1, \ldots, x_n$. Due to orthogonality of the individual component functions, the variance of f will be equal to the sum of variances of each of the individual random variables on the right hand side of equation (1). Usually only the few lowest-order terms have significant contributions to the overall variance of f. HDMR expansions can be used in a broader sense, as the input variables need not be random and one may be interested in more than the variance or some finite moment of the output. They may be used for representing the input–output mapping over the operating region of the input variables. As such, they are multivariate approximation/interpolation schemes as well as a means to analyze the relevant statistics of a random output. The measure μ defined over the input variable

space does not necessarily assume randomness of the input variables. It is rather a "weight" chosen to give different HDMR expansions distinct characteristics that may be useful for a particular representation problem. For example, the ANOVA-HDMR in section 2.1 is useful for measuring the contribution of the variance of individual component functions to the overall variance of the output. On the other hand, a cut-HDMR expansion (section 2.2) is an exact representation of the output $f(x)$ along the hyperplanes passing through a reference point. Thus, the choice of the particular HDMR is suggested by what is desired to be known about the output and is also dictated by the amount and type of available data.

From equation (32) one may show that a compact formulation of the projection operators is given by

$$\begin{aligned} P_{i_1\ldots i_l} f(x) &= \int_{K^n} K_{i_1\ldots i_l}(x;x') f(x')\,\mathrm{d}x', \\ K_0(x;x') &= \prod_{j=1}^{n} g_j\left(x'_j\right), \\ K_{i_1\ldots i_l}(x;x') &= \prod_{j\in\{i_1,\ldots,i_l\}} \left[\delta\left(x_j - x'_j\right) - g_j\left(x'_j\right)\right] \prod_{k\notin\{i_1,\ldots,i_l\}} g_k\left(x'_k\right). \end{aligned} \tag{40}$$

From the analysis above it is evident that the overall form of the HDMR expansion is uniquely defined once the projection operators are specified. For illustration, we present two classes of HDMRs with the projection operators specified below.

2.1. ANOVA-HDMR expansion

In this case, X is defined as the space of square-integrable functions on K^n. The measure μ is taken as the ordinary Lebesgue measure

$$\mathrm{d}\mu(x) = \mathrm{d}x = \mathrm{d}x_1\,\mathrm{d}x_2\ldots\,\mathrm{d}x_n. \tag{41}$$

With this choice, the actions of the projection operators in the ANOVA-HDMR are given by

$$\begin{aligned} f_0(x) \equiv P_0 f(x) &= \int_{K^n} f(x)\,\mathrm{d}x, \\ f_i(x_i) \equiv P_i f(x) &= \int_{K^{n-1}} f(x) \prod_{j\neq i} \mathrm{d}x_j - P_0 f(x), \\ f_{ij}(x_i,x_j) \equiv P_{ij} f(x) &= \int_{K^{n-2}} f(x) \prod_{k\notin\{i,j\}} \mathrm{d}x_k - P_i f(x) - P_j f(x) - P_0 f(x), \\ &\vdots \\ f_{i_1\ldots i_l}(x_{i_1},\ldots,x_{i_l}) \equiv P_{i_1\ldots i_l} f(x) &= \int_{K^{n-l}} f(x) \prod_{k\notin\{i_1,\ldots,i_l\}} \mathrm{d}x_k \end{aligned}$$

$$
\begin{aligned}
&- \sum_{j_1<\cdots<j_{l-1}\subset\{i_1,i_2,\ldots,i_l\}} P_{j_1\ldots j_{l-1}} f(x) \\
&- \sum_{j_1<\cdots<j_{l-2}\subset\{i_1,i_2,\ldots,i_l\}} P_{j_1\ldots j_{l-2}} f(x) - \cdots \\
&- \sum_j P_j f(x) - P_0 f(x),
\end{aligned} \tag{42}
$$

where the kernel functions are given by the expressions

$$
\begin{aligned}
K_0(x;x') &= 1, \\
K_{i_1\ldots i_l}(x;x') &= \prod_{j\in\{i_1,\ldots,i_l\}} \left[\delta\left(x_j - x'_j\right) - 1\right],
\end{aligned} \tag{43}
$$

as a special case of equation (40). The expansion based on these integrals is a multivariate representation of the model output. It is mainly used [5,12,22,24,30] for statistics purposes. If the input consists of independently distributed uniform random variables (corresponding to the ordinary Lebesgue measure above), then the component functions will be uncorrelated and the overall variance of the ANOVA-HDMR can be written as follows:

$$
D \equiv \mathbf{E}(f - f_0)^2 = \sum_i D_i + \sum_{i<j} D_{ij} + \cdots + \sum D_{12\ldots n}, \tag{44}
$$

where the individual variances $D_{i_1\ldots i_l}$ are given by

$$
D_{i_1\ldots i_l} = \int_{K^l} (f_{i_1\ldots i_l})^2 \,\mathrm{d}x_{i_1} \ldots \mathrm{d}x_{i_l}. \tag{45}
$$

Global sensitivity indices based on these variances are defined as [12,22,30]

$$
S_{i_1\ldots i_l} = \frac{D_{i_1\ldots i_l}}{D}, \tag{46}
$$

where $S_{i_1\ldots i_l}$ is the fractional contribution of the input set $\{x_{i_1},\ldots,x_{i_l}\}$ to the variance of the output. Although an ANOVA-HDMR might be used as a multivariate representation of the output, it is most useful as a sensitivity or uncertainty analysis of the model output.

A significant drawback of employing ANOVA-HDMR is the need to compute the above integrals to extract each component function for systems with high dimensions $n \gg 10$. These high-dimensional integrals would likely need to be carried out by Monte-Carlo integration, and a large number of sample points generally will be required to attain good accuracy. The computation of the sensitivities $S_{i_1\ldots i_l}$ requires the generation of $N \times (2n)$ uniformly distributed random numbers and the number of model evaluations needed for Lth-order ANOVA-HDMR is given by

$$
N \times \left(\sum_{i=0}^{L} \frac{n!}{(n-i)!i!} \right), \tag{47}
$$

where N is the sample size for the computation of the each integral in the Lth-order ANOVA-HDMR expansion. Even if $L \ll n$, the cost of such an analysis can be very high as reliable results will often call for $N \gg 10^3$. To circumvent this difficulty, a computationally more efficient cut-HDMR expansion will be introduced in the following section for more general model representation and reexpression into the ANOVA-HDMR form. Finally, although ANOVA-HDMR is often costly, if only the total contribution of each variable x_i to the variance is sought, then a simplification is possible using Monte-Carlo sampling methods [12].

2.2. Cut-HDMR expansion

In this case, X is the space of functions on K^n taking finite value at the point $y = (y_1, y_2, \ldots, y_n)$. The measure μ is taken as the Dirac measure located at the point $y = (y_1, y_2, \ldots, y_n)$, i.e.,

$$\mathrm{d}\mu(x) = \prod_{i=1}^{n} \delta(x_i - y_i)\,\mathrm{d}x_i. \tag{48}$$

The point y will be called the "cut" center. Cut-HDMR is an expression of the function $f(x)$ as a superposition of its values on lines, planes and hyperplanes of higher orders passing through the cut center y. The exploration of the output surface $f(x)$ may be global and the value of y is irrelevant if the expansion is taken out to convergence.

The component functions of $f(x)$ obtained within cut-HDMR are given as follows. The notation $f^{i_1\ldots i_l}(x_{i_1}, \ldots, x_{i_l})$ stands for the function $f(x)$ with all the remaining variables, besides $x_{i_1}, \ldots, x_{i_l}$ of the input vector set to y, e.g., $f^i(x_i)$ stands for $f(y_1, \ldots, y_{i-1}, x_i, y_{i+1}, \ldots, y_n)$:

$$\begin{aligned}
f_0 &= P_0 f(x) = f(y),\\
f_i(x_i) &= P_i f(x) = f^i(x_i) - P_0 f(x),\\
f_{ij}(x_i, x_j) &= P_{ij} f(x) = f^{ij}(x_i, x_j) - P_i f(x) - P_j f(x) - P_0 f(x),\\
&\vdots\\
f_{i_1\ldots i_l}(x_{i_1}, \ldots, x_{i_l}) &= P_{i_1\ldots i_l} f(x) = f^{i_1\ldots i_l}(x_{i_1}, \ldots, x_{i_l})\\
&\quad - \sum_{\{j_1,\ldots,j_{l-1}\}\subset\{i_1,\ldots,i_l\}} P_{j_1\ldots j_{l-1}} f(x)\\
&\quad - \sum_{\{j_1,\ldots,j_{l-2}\}\subset\{i_1,\ldots,i_l\}} P_{j_1\ldots j_{l-2}} f(x) - \cdots\\
&\quad - \sum_{j} P_j f(x) - P_0 f(x),
\end{aligned} \tag{49}$$

with the kernel functions given by the expressions

$$K_0(x;x') = \prod_{j=1}^{n} \delta(x'_j - y_j),$$

$$K_{i_1\ldots i_l}(x;x') = \prod_{j\in\{i_1,\ldots,i_l\}} \left[\delta(x_j - x'_j) - \delta(x'_j - y_j)\right] \prod_{k\notin\{i_1,\ldots,i_l\}} \delta(x'_k - y_k). \quad (50)$$

The computational or experimental cost of generating the cut-HDMR up to the lth level, when it is used for interpolation purposes, is given by

$$\sum_{i=0}^{l} \frac{n!}{(n-i)!i!}(s-1)^i, \quad (51)$$

where s is the number of sample points taken along each axis. If convergence of the cut-HDMR expansion occurs at $L \ll n$, then the sum above is dominated by the Lth term and, considering $s \gg 1$, we get full space resolution at the computational labor of $\sim(ns)^L/L!$. This result is in stark contrast with the conventional view of exponential scaling $\sim s^n$. Applications with well defined physical systems indicate that one may expect $L \sim$ 1–3 for good quality results in many cases. The choice of the cut center y is irrelevant if the cut-HDMR is taken out to acceptable convergence at order L.

As an illustration the cut-HDMR was applied to a 0-D stratospheric chemical kinetics model [26] for an air parcel at 45°N latitude and 20 km altitude. The heterogeneous chemistry model was adapted from the NASA GSFC 2-D atmospheric chemistry model [4,14] to run in 0-D. The model contained 39 chemical species and 106 reactions. The 39 outputs were the concentrations of the chemical species involved and the total number of input variables was 46. These input variables consisted of 39 chemical species, 5 parameters describing the photolysis rates, the number of daylight hours, and temperature. The model is a set of 39 coupled ordinary differential equations (ODEs) for the species. Denoting the concentration of the species at time n by the vector x, the cut-HDMR learned the mapping f as

$$x_{n+1} = f(x_n, \alpha_n), \quad (52)$$

where the vector α denotes the 7 remaining inputs. A selected set of high-quality simulations of the original model were carried out with a standard GEAR integrator to create a cut-HDMR as discrete tables for all the significant expansion functions for each of the 39 output species. The inputs were chosen on a special grid so that they were suitable for learning the mapping by cut-HDMR expansion for a step $x_n \to x_{n+1}$ corresponding to 24 hours taking into account the orthogonality property in equation (10). During this period of 24 hours the parent ODE code took up to ∼2000 time steps to achieve acceptable accuracy. The cut-HDMR expansion for each of the 39 outputs was carried out to second order which was found to give good accuracy. Implementation of this second-order cut-HDMR involved the

interpolation of functions of only one or two variables which is very easy to carry out. We may denote the resulting mapping by f^{cut} and replace the above dynamics by

$$x_{n+1} = f^{\text{cut}}(x_n, \alpha_n). \tag{53}$$

In order to test the accuracy of the mapping f^{cut} in representing the actual mapping f, the evolution of the species was followed for one year by using (1) a GEAR integrator with $\sim$2000 time steps per day, and (2) a HDMR integrator with a time step of one day. The agreement between the HDMR integrator and the GEAR integrator was very good. Both long- and short-time scale species were accurately calculated with the worst case error being only $\sim$2%. The cut-HDMR in equation (53) was then repeatedly applied out to 40 years with completely stable behavior. The inherent mass conserving property of the HDMR in equation (38) is central to this behavior.

The computational savings with the HDMR integrator were determined by observing the execution time of 1000 simulations, each for one day in length, and comparing the timings of the HDMR and GEAR integrators. The analysis was performed with random initial conditions. The HDMR integrator showed dramatic computational savings of greater than $\sim 10^3$ over the GEAR integrator. Such comparisons need to be taken with caution, as tolerance issues also enter. However, attempts at accelerating the GEAR solver by significantly reducing the tolerance resulted in unstable behavior, and the advantage of HDMR remained. Further research needs to explore how HDMR will behave for treating inherently unstable ODEs.

Several relationships exist between ANOVA-HDMR and cut-HDMR. The first of these concerns the relation between the component functions of ANOVA-HDMR and those of cut-HDMR given by

$$f^{\text{anova}}_{i_1 \ldots i_l}(x_{i_1}, \ldots, x_{i_l}) = \int_{K^n} f^{\text{cut}}_{i_1 \ldots i_l}(x_{i_1}, \ldots, x_{i_l})\, \mathrm{d}y, \tag{54}$$

where the integrand is a cut-HDMR expansion function implicitly understood to depend on y. Recall that $f^{\text{cut}}_{i_1 \ldots i_l}$ is exact along the hyperplanes through the cut center y. Thus $f^{\text{anova}}_{i_1 \ldots i_l}$ is good on average throughout the subvolumes K^l, $l \leqslant n$.

Computation of the ANOVA-HDMR expansion of f involves multi-dimensional Monte-Carlo integrations of f which may be costly. If the objective is to compute the ANOVA-HDMR component functions, then an efficient two-step approach can be envisioned as follows (note that computation of cut-HDMR functions requires that the function $f(x)$ be sampled at special points, i.e., it can be computed if one has control over the input variables):

(1) Compute the cut-HDMR component functions and approximate the function $f(x)$ by

$$f(x) \approx f^{\text{cut}}(x) = f_0^{\text{cut}} + \sum_i f_i^{\text{cut}}(x_i) + \sum_{i<j} f_{ij}^{\text{cut}}(x_i, x_j) + \cdots. \tag{55}$$

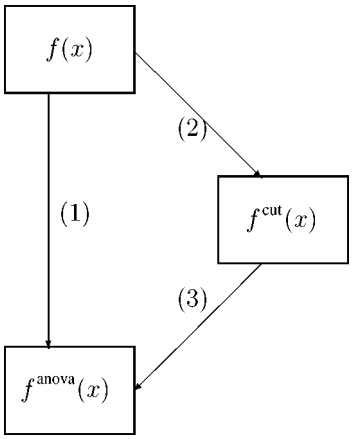

Figure 1. Two equivalent routes to the ANOVA-HDMR. The indirect route through the cut-HDMR is generally more efficient.

(2) Compute the ANOVA-HDMR expansion of $f^{\text{cut}}(x)$. Assuming that an Lth-order cut-HDMR approximates $f(x)$ to good accuracy, then $f^{\text{cut}}(x)$ will consist of a superposition of functions of at most L variables. When $L \ll n$, quadrature techniques can be used for the integrations of the function $f(x)$ to compute the ANOVA-HDMR functions in a computationally accurate and efficient way.

A graphical representation of the above scheme is shown in figure 1.

If the cut-HDMR approximates $f(x)$ to good accuracy at the Lth order, then the computation route (2) + (3) in figure 1 will give a very close approximation to the true $f^{\text{anova}}(x)$ and the computational effort required to construct the $f^{\text{anova}}(x)$ will be much less. The computational cost of generating the Lth-order cut-HDMR is given by equation (51). In contrast, the number of model evaluations for the Lth-order ANOVA-HDMR is given by equation (47). Thus the ratio of the computational cost of cut-HDMR to that of ANOVA-HDMR is given by

$$\rho \equiv \frac{\sum_{i=0}^{L} \frac{n!}{(n-i)!i!} \frac{(s-1)^i}{N}}{\sum_{i=0}^{L} \frac{n!}{(n-i)!i!}}. \tag{56}$$

The condition $(s-1)^L < N$ ensures that the ratio ρ is less than 1. Assuming that cut-HDMR converges at low order ($L \sim$ 1–3), then the ratio will satisfy $\rho \ll 1$ observing that typically $s \sim 10$ and $N \gg 10^3$. Computation of ANOVA-HDMR using route (3) in figure 1 after obtaining $f^{\text{cut}}(x)$ is straightforward involving integrals of dimensions no larger than L. Since L is assumed to be small on physical grounds, the integrations can be carried out very accurately via quadrature methods with only a few points, while using Monte-Carlo integration directly in ANOVA-HDMR to the same accuracy will call for a very large number of points N. In general, the savings arise as (1) calls for integrations over f of dimensions $n, n-1, \ldots, n-L$. In contrast, (2) calls for no integrations and (3) only calls for integrations of dimensions $1, 2, \ldots, L$ and we expect

that $L \ll n$. For $n \gg 1$, the integration by path (1) would need to be carried out by costly statistical sampling (e.g., Monte-Carlo), while the integrals in step (3) of the alternate route for a typical case of $L \leqslant 3$ can accurately be performed by quadrature. It is evident that the dimension of the integrals to compute via steps (2) and (3) is the complement of those via step (1).

3. Functional HDMR

If the inputs to the physical system consist of a set of functions, then the physical model output now becomes a functional. We assume that these functionals are defined on the product space $C^n[0,1]$, where $C[0,1]$ denotes the space of continuous functions on the unit interval. Thus an element $x(t) \in C^n[0,1]$ is a vector function of the form

$$x(t) = \big(x_1(t), x_2(t), \ldots, x_n(t)\big), \quad x_i(t) \in C[0,1]. \tag{57}$$

One approach to this functional mapping problem is to assume that a discretization of the following form is valid:

$$x_i(t) \approx \sum_{k=1}^{N_i} c_{ik}\phi_k(t), \tag{58}$$

where $\{\phi_k(t)\}$ is a family of orthogonal functions with either global or local support. Then, any "functional" defined on $C^n[0,1]$ becomes a "function" of the parameters c_{ik} and the function HDMR in section 2 can be used to learn the functional mapping. This approach has been successfully implemented for an atmospheric radiative heating problem [27] where the input consisted of species and temperature profiles as a function of altitude. If each $x_i(t)$ is a stochastic process, then the distribution of the random variables c_{ik} would be specified from the distribution of input functions. This discretization of the input functions can result in many variables which under some conditions may be difficult to interpret physically. A different approach may be taken to directly generate a *functional* analog of the HDMR expansion. We defined the function HDMR expansions in terms of projection operators whose action was expressed as integrals over the output model function. A direct generalization to a functional HDMR expansion requires the definition of a functional integral on the particular function space from which the output is drawn. In many respects, functional HDMR has features analogous to function HDMR and the similarity will be exploited in the development below.

A measure μ on the space $C^n[0,1]$ of vector functions $x(t) \equiv [x_1(t), x_2(t), \ldots, x_n(t)]$ is completely specified by its definition on the sets of the form

$$Q_{t_1 t_2 \ldots t_k}(B) = \big\{x(\cdot) \in C^n[0,1]\colon\ \big(x(t_1), x(t_2), \ldots, x(t_k)\big) \in B \subset R^{n\times k}\big\}, \quad t_i \in [0,1], \tag{59}$$

where B is a Borel subset of $R^{n\times k}$. We also denote by $\mathcal{L}(C^n[0,1])$ the space of functionals on $C^n[0,1]$ which are not necessarily linear. Having equipped the space

$C^n[0,1]$ with the measure μ, we denote the integral of a functional $F[\cdot]$ on $C^n[0,1]$ as $\int F[x]\,\mathcal{D}\mu(x)$.

Joint distributions of the subsets of the input vector $x(t)$ are specified by measures $\mu_{i_1\ldots i_l}(x)$ which are defined on sets of the form

$$Q^{i_1 i_2\ldots i_l}_{t_1 t_2\ldots t_k}(B) = \big\{x_{i_1\ldots i_l}(\cdot)\in C^l[0,1]\colon\ \big(x_{i_1\ldots i_l}(t_1),\ldots,x_{i_1\ldots i_l}(t_k)\big)\in B\subset R^{l\times k}\big\},\quad t_i\in[0,1], \tag{60}$$

where we use the notation $x_{i_1\ldots i_l}(t)\equiv(x_{i_1}(t),x_{i_2}(t),\ldots,x_{i_l}(t))$. In this case, integrals of a functional $F[\cdot]$ with respect to the input vector $x_{i_1\ldots i_l}(t)$ are denoted by $\int F[x]\,\mathcal{D}\mu_{i_1\ldots i_l}(x)$, where F is any functional defined on $C[0,1]$.

We assume that the inputs are independent of each other and the measure μ has the following properties:

$$\mathcal{D}\mu(x)\equiv\mathcal{D}\mu(x_1,\ldots,x_n)=\prod_{i=1}^{n}\mathcal{D}\mu_i(x_i),\qquad \int_{C[0,1]}\mathcal{D}\mu_i(x_i)=1. \tag{61}$$

The inner product $\langle\cdot,\cdot\rangle$ on $\mathcal{L}(C^n[0,1])$ induced by the measure μ is defined as follows:

$$\langle F,H\rangle\equiv\int F[x]H[x]\,\mathcal{D}\mu(x),\qquad F[x],H[x]\in\mathcal{L}\big(C^n[0,1]\big). \tag{62}$$

Two functionals $F[x]$ and $H[x]$ will be called orthogonal if $\langle F,H\rangle=0$. Note that functionals $F[x]$ and $H[x]$ may have different sets of input functions. The norm $\|\cdot\|$ on $\mathcal{L}(C^n[0,1])$ induced by the above inner product is defined as follows:

$$\|F\|\equiv\big(\langle F,F\rangle\big)^{1/2}\equiv\left(\int F^2[x]\,\mathcal{D}\mu(x)\right)^{1/2}. \tag{63}$$

Given these relations, we define the following decomposition of $\mathcal{L}(C^n[0,1])$ and associated projection operators corresponding to each subspace:

Definition. $\mathcal{V}_0,\{\mathcal{V}_i\},\{\mathcal{V}_{ij}\},\ldots,\mathcal{V}_{12\ldots n}\subset\mathcal{L}(C^n[0,1])$ are defined as follows:

$$\mathcal{V}_0\equiv\big\{F\in\mathcal{L}\big(C^n[0,1]\big)\colon\ F=C,\ \text{where } C\in R \text{ is a constant}\big\},$$

$$\mathcal{V}_i\equiv\left\{F\in\mathcal{L}\big(C^n[0,1]\big)\colon\ F=F_i[x_i]\text{ is a functional of only the input } x_i(t)\text{ with }\int_{C[0,1]}F\,\mathcal{D}\mu_i(x_i)=0\right\},$$

$$\mathcal{V}_{ij}\equiv\left\{F\in\mathcal{L}\big(C^n[0,1]\big)\colon\ F=F_{ij}[x_i,x_j]\text{ is a functional of only the inputs } x_i(t)\text{ and }x_j(t)\text{ with }\int_{C[0,1]}F\,\mathcal{D}\mu_k(x_k)=0,\ k=i,j\right\},$$

$$\vdots$$

$$\mathcal{V}_{i_1\ldots i_l} \equiv \Big\{ F \in \mathcal{L}\big(C^n[0,1]\big)\colon\ F = F_{i_1\ldots i_l}[x_{i_1},\ldots,x_{i_l}] \text{ is a functional of only the inputs } x_{i_1}(t),\ldots,x_{i_l}(t) \text{ with } \int_{C[0,1]} F\,\mathcal{D}\mu_k(x_k) = 0,\ k = i_1,\ldots,i_l \leqslant n \Big\},$$

$$\vdots$$

$$\mathcal{V}_{12\ldots n} \equiv \Big\{ F \in \mathcal{L}\big(C^n[0,1]\big)\colon\ F = F_{12\ldots n}[x_1,\ldots,x_n] \text{ with } \int_{C[0,1]} F\,\mathcal{D}\mu_k(x_k) = 0,\ k = 1,2,\ldots,n \Big\}. \tag{64}$$

The integral constraints in equation (64) are chosen to assure the orthogonality of the functionals $\{F_{i_1\ldots i_l}\}$.

Lemma 1. The following proposition can be deduced immediately from the definition above: $\mathcal{L}(C^n[0,1])$ is the direct sum of the subspaces defined above, i.e.,

$$\mathcal{L}\big(C^n[0,1]\big) = \mathcal{V}_0 \oplus \sum_i \mathcal{V}_i \oplus \sum_{i<j} \mathcal{V}_{ij} \oplus \cdots \oplus \sum_{i_1<\cdots<i_l} \mathcal{V}_{i_1\ldots i_l} \oplus \cdots \oplus \mathcal{V}_{12\ldots n}, \tag{65}$$

where $\oplus$ denotes the direct sum operator. The corollary to this proposition is that $F[x] \in \mathcal{L}(C^n[0,1])$ can be written as

$$F[x] = F_0 + \sum_i F_i[x_i] + \sum_{i<j} F_{ij}[x_i,x_j] + \cdots + \sum_{i_1<\cdots<i_l} F_{i_1\ldots i_l}[x_{i_1},\ldots,x_{i_l}] + \cdots + F_{12\ldots n}[x_1,x_2,\ldots,x_n]. \tag{66}$$

Decomposition (65) of $\mathcal{L}(C^n[0,1])$ is unique subject to the choice of measure μ, which, in turn, implies that expansion (66) is unique. The proof is the same as in the function HDMR case.

Lemma 2. Decomposition (65) suggests the following family of projection operators:

$$\begin{aligned}
F_0 \equiv P_0F(x) &= \int_{C^n[0,1]} F[x]\,\mathcal{D}\mu(x),\\
F_i[x_i] \equiv P_iF(x) &= \int_{C^{n-1}[0,1]} F[x]\,\mathcal{D}\mu_i(x) - P_0F[x],\\
F_{ij}[x_i,x_j] \equiv P_{ij}F(x) &= \int_{C^{n-2}[0,1]} F[x]\,\mathcal{D}\mu_{ij}(x) - P_iF[x] - P_jF[x] - P_0F[x],\\
&\vdots
\end{aligned}$$

$$F_{i_1\ldots i_l}[x_{i_1}\ldots x_{i_l}] \equiv P_{i_1\ldots i_l}F[x] = \int_{C^{n-l}[0,1]} F[x]\,\mathcal{D}\mu_{i_1 i_2\ldots i_l}(x) - \sum_{j_1<\cdots<j_{l-1}\subset\{i_1,\ldots,i_l\}} P_{j_1\ldots j_{l-1}}F[x] - \sum_{j_1<\cdots<j_{l-2}\subset\{i_1,\ldots,i_l\}} P_{j_1\ldots j_{l-2}}F[x] - \cdots - \sum_j P_j F[x] - P_0 F[x]. \tag{67}$$

These operators are chosen so that the variational problem

$$\min_u \big\|F(x)-u\big\|, \quad u\in \mathcal{V}_0 \oplus \sum_i \mathcal{V}_i \oplus \sum_{i<j}\mathcal{V}_{ij} \oplus \cdots \oplus \sum_{i_1<\cdots<i_l}\mathcal{V}_{i_1\ldots i_l} \tag{68}$$

is minimized with

$$u = \left(P_0 + \sum_i P_i + \sum_{i<j} P_{ij} + \cdots + \sum_{i_1<\cdots<i_l\subset\{1,2,\ldots,n\}} P_{i_1 i_2\ldots i_l}\right)F[x]. \tag{69}$$

The proof of equation (69) is the same as in the function HDMR case.

The functional projection operators have the same properties as the function HDMR projection operators. The first term in equation (66) above is the zeroth-order functional HDMR approximation to the functional. The next set of terms containing $F_i[x_i]$ gives the independent functional action of $x_i(t)$. The first two terms constitute the first-order HDMR approximation, etc. The last functional $F_{12\ldots n}[x_1, x_2, \ldots, x_n]$ gives any residual nth-order correlations amongst the functions upon the output. Each of the integrals above can be computed by Monte-Carlo simulations given the distribution μ.

For the ease of illustration, throughout the rest of the discussion, we will assume that the input functions to the system are independent Wiener processes on time segment $[0, 1]$. A Wiener, or Brownian motion, process is a random Gaussian process with zero mean and correlation function $R(t, s) = \min(t, s)$, which is a model of a suitable physical phenomenon, i.e., the Brownian motion. An n-dimensional Wiener process is defined as a vector process

$$W \equiv \big[W_1(t), W_2(t), \ldots, W_n(t)\big], \tag{70}$$

where the one-dimensional processes $\{W_i(t)\}_{t\geqslant 0}$ are independent Wiener processes.

Let $F[W]$ denote some functional of the vector process $W = [W_1(t), W_2(t), \ldots, W_n(t)]$ and let μ denote the Wiener measure defined on the product space $C = C^n[0, 1]$. By $\int_C F[W]\,\mathcal{D}\mu(W)$ we denote the integral of the functional $F[W]$ with respect to the Wiener measure μ (see the appendix).

As an illustration consider the first-order functional HDMR approximation to the following functional:

$$F\big[W_1(t), W_2(t)\big] = \int_0^1 W_1^2(t)\,\mathrm{d}t + \alpha\bigg[\int_0^1 W_1(t)W_2(t)\,\mathrm{d}t\bigg]^2 + \int_0^1 W_2^4(t)\,\mathrm{d}t. \quad (71)$$

Employing the material in the appendix, we get the following component functions:

$$\begin{aligned} F_0 &= \frac{13}{12} + \frac{\alpha}{6}, \\ F_1\big[W_1(t)\big] &= \int_0^1 W_1^2(t)\,\mathrm{d}t + 2\alpha\int_0^1\int_0^t sW_1(t)W_1(s)\,\mathrm{d}t\,\mathrm{d}s + \frac{7}{12} - F_0, \\ F_2\big[W_2(t)\big] &= \int_0^1 W_2^4(t)\,\mathrm{d}t + 2\alpha\int_0^1\int_0^t sW_2(t)W_2(s)\,\mathrm{d}t\,\mathrm{d}s + \frac{1}{2} - F_0. \end{aligned} \quad (72)$$

Various values of the constant α will be used to understand the effect of the interaction term. Functional HDMR was applied to the above model at first order. Since the above functionals represent a random variable, the statistics of the following error measure represent the goodness of the functional HDMR approximation:

$$\varepsilon \equiv \left\{\left|\frac{F - F^{\mathrm{HDMR}}}{F}\right|\right\}, \quad (73)$$

where $F^{\mathrm{HDMR}} = F_0 + F_1[W_1(t)] + F_2[W_2(t)]$. The error ε is considered a vector of length 1000 corresponding to the number of runs with random input functions $W_1(t)$ and $W_2(t)$. The criterion in (73) can be misleading at the points where the model output is close to zero; we observed large outliers in the 1000-sample Monte-Carlo runs. The frequency of these large values is recorded and the following redefined error vector $\widehat{\varepsilon}$ is employed:

$$\widehat{\varepsilon} \equiv \{\varepsilon_i\colon\ \varepsilon_i < 1\} \quad (74)$$

along with an observation of its length L[$\widehat{\varepsilon}$]. The length of the vector is a measure of the domain where the relative error is smaller than one. Table 1 lists α and the associated mean (M), standard deviation (SD) about the mean of the above vector $\widehat{\varepsilon}$, and the length of $\widehat{\varepsilon}$. The accuracy of the first-order HDMR approximation decreases as the coefficient α increases consistent with the contribution of the interaction term to the overall functional.

Table 1
Accuracy of the first-order functional HDMR.

	$\alpha = 0.5$	$\alpha = 1.0$	$\alpha = 5.0$
M[$\hat{\varepsilon}$]	0.1087	0.1686	0.3032
SD[$\hat{\varepsilon}$]	0.1538	0.1986	0.2458
L[$\hat{\varepsilon}$]	988	943	745

3.1. Functional cut-HDMR

The computation of the integrals in equation (67) is expensive. Instead of averaging, a single run of the multi-dimensional vector $x = (x_1(t), x_2(t), \ldots, x_n(t))$ can be used to formulate a functional cut-HDMR expansion which is an analog of the cut-HDMR expansion presented in section 2.2. Let $y \equiv [y_1(t), y_2(t), \ldots, y_n(t)]$ be the reference function vector used for expansion. The choice of y typically would be made on physical grounds as a rational reference for the system, although this choice is irrelevant when the HDMR is taken out to a practical level of convergence. Before considering the projection operators for the cut-functional HDMR, we fix some notation. $F^{i_1 i_2 \ldots i_l}[x_{i_1}, \ldots, x_{i_l}]$ stands for the functional $F[x]$ with all the remaining input functions set to reference vector function y, e.g., $F^i[x_i]$ stands for the expression $F[y_1(t), \ldots, y_{i-1}(t), x_i(t), y_{i+1}(t), \ldots, y_n(t)]$.

The projection operators associated with functional cut-HDMR take the following form:

$$
\begin{aligned}
F_0 &= P_0 F[x] = F[y], \\
F_i[x_i] &= P_i F[x] = F^i[x_i] - P_0 F[x], \\
F_{ij}[x_i, x_j] &= P_{ij} F[x] = F^{ij}[x_i, x_j] - P_i F(x) - P_j F[x] - P_0 F[x], \\
&\vdots \\
F_{i_1 \ldots i_l}[x_{i_1}, \ldots, x_{i_l}] &= P_{i_1 \ldots i_l} F[x] = F^{i_1 \ldots i_l}[x_{i_1}, \ldots, x_{il}] \\
&\quad - \sum_{j_1 < j_2 < \cdots < j_{l-1} \subset \{i_1, i_2, \ldots, i_l\}} P_{j_1 j_2 \ldots j_{l-1}} F[x] \\
&\quad - \sum_{j_1 < j_2 < \cdots < j_{l-2} \subset \{i_1, i_2, \ldots, i_l\}} P_{j_1 j_2 \ldots j_{l-2}} F[x] - \cdots \\
&\quad - \sum_j P_j F[x] - P_0 F[x].
\end{aligned} \tag{75}
$$

The relationship summarized by figure 1 is valid between general functional HDMR and the special case of functional cut-HDMR, i.e., the functional cut-HDMR can be used to compute other functional HDMR expansions of the functional $F[x]$.

As an illustration, we give the following example:

$$
F\big[W_1(t), W_2(t), W_3(t)\big] = \exp\left[\int_0^1 \big(W_1(t)\big)^2 \, \mathrm{d}t + \alpha \int_0^1 W_2(t) W_3(t) \, \mathrm{d}t \right]. \tag{76}
$$

The coefficient α weighs the importance of the interaction term. This functional is highly nonlinear due to the exponential behavior. The same error criterion in equation (73) is also employed in table 2. As expected, the accuracy of the first-order functional cut-HDMR diminishes as the value of α increases.

Table 2
Accuracy of the first-order functional cut-HDMR.

	$\alpha = 0.1$	$\alpha = 0.5$	$\alpha = 1.0$
M[$\hat{\varepsilon}$]	0.0414	0.1668	0.3097
SD[$\hat{\varepsilon}$]	0.0445	0.1712	0.2548
L[$\hat{\varepsilon}$]	1000	995	903

4. Applications of HDMR

The HDMR technique is a tool to enhance modeling or an experimental effort where the interest centers on the input–output relationships. There is a broad family of applications to exploit the HDMR capabilities. Presently, applications have been made to chemical kinetics [26], radiative transport [27], materials discovery [21,25] and statistical analysis [22,30]. Some of the applications discussed below go beyond those currently available. The particular applications of HDMR discussed below are not exhaustive and they should be regarded as representative.

4.1. Fully equivalent operational models

All the HDMR applications in sections 4.2–4.7 are associated with exploring the role and relationships amongst the model variables. An application of HDMR, to some degree underlying the ability to execute the other applications in sections 4.2–4.7, is model component replacement by highly efficient equivalent forms. This operation takes advantage of the fact that complex models are typically broken into various components (e.g., involving chemistry, mechanical coupling, mass transport, etc.). These components of an overall model are often treated by numerical splitting techniques, thus isolating them for efficient replacement with equivalent HDMRs. Some components (e.g., radiation transport in weather modeling) can be exceedingly costly contributions to the computational effort as they correspond to high overhead operations which are repeated many times in the course of model execution. In some applications, the model "component" may be the entire model. The input–output space can be of high dimension n, but typically it is expected to have systematic structure. Thus, one could envision "learning" the model input–output behavior through the observation of model runs for subsequent encapsulation of the information into an HDMR expansion. Once the expansion functions f_0, f_i, f_{ij}, etc. are learned, they may be reused as a basis to predict output behavior at any other point x in the space called upon in additional execution of the model. The HDMR expansion obtained in this way corresponds to a fully equivalent operational model (FEOM) which could replace the original one (i.e., the model component(s)). The logic will be most appropriate for model components that involve very large numbers of computational operations which are repeated many times in executing the overall model. The computational savings using a FEOM can be dramatic. A study on atmospheric radiation transport treating water vapor, and temperature as input column functions led to a computational saving by a factor of

$\sim 10^3$ for the atmospheric heating rate with errors no larger than a few percent at all altitudes [26]. In an additional study discussed in section 2.2, a FEOM acted as an integrator of a set of coupled ordinary differential equations describing atmospheric chemical kinetics. In this case, the FEOM variables $(x_1, x_2, \ldots, x_N)$ consisted of the initial conditions for the system of equations and the outputs were the species at 24 hours later. High-quality results were produced over an interval of many years by repeated use of the FEOM from one day to the next at computational savings of $\sim 10^4$ over the original GEAR code while maintaining very good accuracy. In general, the method may be applied to an autonomous set of differential equations of the form

$$\dot{x} = h(x), \quad x(t_0) = x_0. \tag{77}$$

After an appropriate discretization over the vector of input variables x_0, the dynamics of above system can be approximated by a discrete map of the form

$$x_{m+1} = H(x_m), \quad m = 0, 1, 2, \ldots, \tag{78}$$

or, equivalently,

$$x_m = H^m(x_0), \quad m = 1, 2, \ldots, \tag{79}$$

where m indicates the time discretization. Importantly, the map can be discretized on steps much larger than traditional integrator time-steps (cf. the 24-hour HDMR steps mentioned above, while the GEAR integration took $\sim$2000 steps over one day). The map H can be approximated by a cut-HDMR representation and it can be repeatedly used as an integrator of the dynamical system. The behavior of the HDMR approximation to the discrete map when the system exhibits chaotic or possibly other types of unstable behavior is an open question.

The use of FEOMs has potentially broad applicability in many areas and, importantly, the FEOM replacement of a model component (e.g., radiation transport) can be handled as a simple swap for an existing routine without alteration of the remainder of the code. The original model component would likely still be retained, but only called upon if a new required input point x fell outside of the regime explored in generating the FEOM or if the FEOM prediction is estimated to have significant errors. In this case, the output from the new model component run would also serve to enhance the FEOM for its further use. Following this logic, the creation of a FEOM for model component replacement could be performed as a background operation, while the parent code is being exercised in a normal fashion. The latter approach would correspond to generating a FEOM from a space of variables x chosen with a probability distribution dictated by the physical model.

4.2. Identification of key variables and their interrelationships

The terms in the HDMR expansion can be regarded as the generalized sensitivities of the output function $f(x_1, x_2, \ldots, x_n)$ with respect to groups of variables. Each of the functions $f_i(x_i), f_{ij}(x_i, x_j), \ldots$ reveals a unique contribution of the variables

separately or cooperatively to influence the output f. These comments apply to any of the HDMR expansions and the choice of the expansion can give different physical interpretation and quantitative measures of the variable cooperativity. The choice of HDMR expansion to employ will often be guided by physical considerations. For example, if a clear reference state y exists, then the cut-HDMR is natural for variable analysis in relation to y. If statistical variance analysis is needed, then ANOVA-HDMR is appropriate [22,30] as discussed in section 4.3. An example in a study of atmospheric radiation transport [27] involved a functional cut-HDMR expansion of the output atmospheric heating rate with respect to the input column densities of chemical species. Discretization of the functions led to 62 input variables, but the HDMR expansions revealed that many variables were important acting independently and only a modest number of pair correlated contributions existed. Techniques from traditional gradient-based sensitivity analysis can reveal similar relationships [1,2,19,20], but only over small operating uncertainty or scenario variations around a nominal set of conditions. In contrast, the HDMR expansion puts no restrictions on the magnitude, shape or variable range of the individual expansion functions, to reveal the true underlying variable relationships.

4.3. Global uncertainty assessments

Expressing the output uncertainty in terms of model input uncertainty has been a topic of prime interest in virtually all areas of modeling. Monte-Carlo sampling [28] and perturbative sensitivity analysis [19,20] are the traditional approaches to these problems. In both cases, a probability measure is defined on R^n and the goal is to calculate the mean $\bar{f} = \mathbf{E}f$ and standard deviation $\sigma_f = \mathbf{E}(f - \bar{f})^2$ of the output f, as well as to reveal the contributions from the various input variables and their interrelationships. One may show that the ANOVA-HDMR expansion has a direct statistical correlation interpretation [22,30]. Each term of the expansion is associated with a particular contribution to the variance of the output. Orthogonality of the individual terms ensures this behavior. The overall variance σ_f can be written as follows:

$$\begin{aligned}
\sigma_f &= \sum_i \sigma_i + \sum_{i<j} \sigma_{ij} + \cdots, \\
\sigma_i &= \int f_i^2(x_i)\, \mathrm{d}\mu(x_i), \\
\sigma_{ij} &= \int f_{ij}^2\, \mathrm{d}\mu_i(x_i)\, \mathrm{d}\mu_j(x_j), \\
&\vdots
\end{aligned} \tag{80}$$

Monte-Carlo integration [28] would be a means for evaluating above integrals. Another approach would be to use the alternate route in figure 1 which is computationally less expensive. Illustrations of these uncertainty analyses have been made for applications to environmental modeling [22]. The information gained from the decomposition of

the variance σ_f into its subcomponents σ_i, σ_{ij}, etc. can be most valuable for attaining a physical understanding of the origins of uncertainty.

4.4. Quantitative risk assessment

Environmental, industrial, and economic modeling often are performed for the ultimate purpose of providing an assessment of the risk associated with some action that is subject to remediation. There is a serious need for more quantitative and efficient means of performing these assessments. For a quantitative risk assessment, it is generally necessary to split the original set of input variables into two components $(x_1, \ldots, x_s;\, y_1, \ldots, y_r;\, r + s = N)$, where the set $\{x_i\}$ will be referred to as scenario variables under human control (e.g., industrial emissions, etc.) and the set $\{y_j\}$ will correspond to all other model variables (e.g., chemical rates, transport coefficients, mechanical properties, etc.) which are present and subject to some degree of uncertainty. Typically, risk is associated with identifying whether the output exceeds (or goes below) a critical value $f > f_c$. The risk R is defined as the probability $P(f > f_c)$ for this event to occur while simultaneously taking into account the uncertainty amongst the model variables $\{y_j\}$. Thus the risk is defined as

$$R = \int \mathrm{d}\mu(x)\, \mathrm{d}\nu(y)\, H\big[f(x;y) - f_c\big], \tag{81}$$

and the variance of the risk is

$$\sigma_R = -R^2 + \int \mathrm{d}\nu(y)\, \mathrm{d}\mu(x)\, \mathrm{d}\mu(x')\, H\big[f(x;y) - f_c\big] H\big[f(x';y) - f_c\big], \tag{82}$$

where the distribution of the variable group y is given by ν and $H(z)$ is the Heaviside function. We may take special advantage of the HDMR expansion in evaluating the risk and the variance around the risk in a quantitative fashion. These tasks are facilitated by the ability to rapidly evaluate $f(x;y)$. In addition, it will be possible to determine the portion of the scenario variables $(x_1, \ldots, x_r)$ which contribute independently or in a correlated fashion to the risk (cf. section 4.2 above). The analysis will not only provide the risk R, but also a quality assurance on the risk through its variance σ_R due to the model variables $\{y_j\}$ and their uncertainty.

4.5. Inverse problems

Information on the input variables of an input–output relationship is often incomplete. If the objective is to gain knowledge about these unknown input variables from the available output data, the task becomes an inverse problem. This problem is typically ill-posed [34] in the sense that there are usually more unknowns than available measurements. In addition, measurements (i.e., function(al)s of the outputs) will inevitably contain errors and this further contaminates the quality of the quantity to be extracted. These issues are typically dealt with through regularization based on a local

linear sensitivity analysis mapping between the data-model deviations and the sought-after input variables [11,34]. The linearization is an approximation to the true model and can lead to algorithmic instabilities and even a false solution. For inversion applications, the HDMR expansion needs to be extended to consider the case of multiple outputs $f^l(x_1, x_2, \ldots, x_n)$ labeled by the index $l = 1, 2, \ldots$. This index corresponds to distinct observations (e.g., chemical species as well as their spatial locations and/or temporal behavior). The forward problem consists of expressing $f^1, f^2, \ldots$ in terms of the input $x_1, x_2, \ldots, x_n$. The inverse problem is to map the data back to identify the input variables. By reversing the roles of the f's and x's, one can construct an inverse-HDMR expansion for x's in terms of f's. A regularization functional also can be introduced if there is *a priori* knowledge of the input variables to be inverted. An open question is how to express the HDMR expansion of the inverse map in terms of the HDMR expansion of the forward map and analyze the relation between the convergence behaviors of the two expansions.

4.6. Financial and econometrics applications

For many financial applications, one wishes to relate (regress) a response y_t to several variables $x_{1t}, \ldots, x_{lt}$ (t signifies the time component of the financial or econometrics data). Parametric regression models take the form $y_t = f(\Theta; x_{1t}, \ldots, x_{lt})$, where the form of the function f is known and the parameter set Θ is to be estimated by satisfying some optimization criteria. Nonparametric regression of y_t takes the form $y_t = f(x_{1t}, \ldots, x_{lt})$ with an unknown function f. Modelling with nonlinear nonparametric regression is normally viewed as computationally very intensive due to the curse of dimensionality mentioned before. Sampling the input space is of exponential cost in the number of input variables. Various learning algorithms have been devised to model the output to good accuracy while being computationally cheaper than a full sampling of the space. Nonparametric regressive schemes include *average derivative estimators* [31], *artificial neural networks* [35], *radial basis function interpolators* [18] and *projection pursuit regression* [7]. A disadvantage of these nonlinear models is that there is no widely accepted procedure for choosing a specific model over another. *A priori* knowledge of the system to be modeled is crucial to the success of the model. HDMR is a nonparametric nonregressive model and as such it has advantages for direct applications to problems in finance and time series econometrics. One possible application is the modelling of the price of financial securities which are dependent on several factors, i.e., parameters of the stochastic differential equation governing the evolution of the price, interest rate, time to maturity of the security and other factors specific to the pay-off structure of the particular security.

4.7. Laboratory applications of HDMR

In many cases, the performance of laboratory or field experiments is done for the explicit purpose of exploring broad regions of the input variable space. Applications of this type abound in many areas including industrial processes, environmental studies,

materials design, engineering control, etc. The most challenging and interesting of these problems arises when the dimension n of the space of inputs is large. This task may be recognized as the learning of the output mapping $f:\Omega \rightarrow R$, where Ω is the space of input values. Traditional statistical sampling techniques, including factorial design, are inadequate as they provide no guidance based on the system behavior. In this case, the notion of the "model" in the HDMR sense is understood to mean the realization of laboratory or field experiments and representing them in a logical fashion to provide an efficient and thorough sampling for analysis of the results. Given the above objective the HDMR expansion provides an ideal approach. When the HDMR expansion converges at low orders, the original NP-complete problem is reduced to one of polynomial scaling in the dimension of the input space. As experiments can be exceedingly expensive to perform, this savings can be critical. One particular application of the cut-HDMR has been made for semiconductor electronic band gap as the observable material property with the input variables being the material compositions. It was shown that the band gap of the material $Ga_{\alpha}In_{1-\alpha}P_{\beta}As_{1-\beta}$ could be reliably described as a function of α and β by a first-order cut-HDMR centered at $\alpha = 0$, $\beta = 0$ corresponding to laboratory band gap input variables for the materials $Ga_{\alpha}In_{1-\alpha}As$ and $InP_{\beta}As_{1-\beta}$. In this case, $n = 2$, and this is a modestly "high-dimensional" semiconductor system. Although each application will have its own features, the domain of combinatorial synthesis poses an intriguing opportunity, as in most realistic cases one has $n \gg 1$ and there very likely will be correlated behavior amongst the input materials or chemical variables. One could envision active feedback between the ongoing experiments and the development of an HDMR to guide the subsequent experiments to rapidly converge on the desired library of materials or compounds for application purposes [21].

5. Conclusion

In this paper, we introduced a family of nonparametric multivariate approximation/interpolation schemes for physically based function(al)s with a large number of input variables. A specific form of the high-dimensional model representations (HDMR) reveals the correlations among the input variables as reflected upon the model output and the nature of the metric in the variable space. Each component function in an HDMR gives the specific contribution of an input or a set of inputs to the output. The HDMRs are useful if they can represent the output to good accuracy at sufficiently low orders. As argued in the text, for most well-defined physical systems, high-order correlated behavior of the input variables is expected to be weak and HDMRs are designed to capture this effect. It is interesting that the greatest body of evidence supporting this statement comes from the multivariate statistical analysis of many systems where rarely more than covariances are needed to capture the physical behavior.

General HDMR expansions are similar in form to the ANOVA expansion used in statistics to analyze the variance of a physical quantity. HDMR is a hierarchical description of the multivariate function $f(x)$ as a sum of component functions of

fewer variables. HDMR does not assume an *a priori* parametric form and as such it is not a fitting algorithm like other regressive multivariate approximation schemes. As shown in section 2, the HDMR functions are optimal with respect to a suitably defined norm with the optimality criterion being a quadratic cost functional. However, the HDMR avoids an explicit optimization (fitting) procedure to represent the output function $f(x)$. For example, the cut-HDMR approach only calls for evaluation of the output on "specified" lines, planes and hyperplanes of higher dimensions to construct expansion (1).

The high computational or experimental effort for representing multivariate functions was one of the motivations of the present work. Without *a priori* information on the nature of the output, multivariate function approximations suffer from the *curse of dimensionality*. Sampling in the n-dimensional space scales exponentially with the dimension n. The number of samples needed to achieve a given degree of accuracy depends on the dimension of the input vector and the smoothness of the function to be approximated. Without any regularization of the output function, one needs s^n sample points to approximate/interpolate the function to a resolution of $1/s$. Therefore, for physical systems with many input variables, a blind reconstruction of the output function $f(x)$ from its sample values is virtually impossible. In this respect, one should consider the storage and computational limitations in constructing $f(x)$. If the time required to obtain a single value of the output is sufficiently fast, representation of the multivariate output may not be difficult. However, when this time is of the order of minutes or larger for a computational model, then representation of the output in high dimensions becomes impossible unless some regularization on the output is imposed. The regularization implicity imposed by HDMR is that the high-order correlated effects of the inputs upon the output are negligible for well-posed physical systems. Similar comments apply for representing the input–output behavior of experimental systems where the curse of dimensionality can be even more critical.

A number of multivariate approximation schemes exist to circumvent this curse of dimensionality. They are inspired by a theorem of Kolmogorov, which states that any multivariate function can be written as a superposition of functions of a suitable set of variables. In the introduction we mentioned three of these approximation schemes collectively known as *learning networks*. Each of these schemes can be preferred over another for a specific problem, however, there are no general rules that determine which one is suitable for a specific problem. The HDMR expansions are based on a general ansatz that for physical systems the *order* of cooperativity amongst the input variables upon the output does not significantly increase as the number of inputs goes up. Consistent with this ansatz, it has been observed in cases of diverse physical phenomena that the first few lowest-order interaction terms are often enough to approximate the output to good accuracy. The computational advantage gained by HDMR (when it converges at low order) is significant. Assuming that a second-order HDMR is an accurate representation of the output, the computational complexity scales quadratically with the number of input variables. Although a thorough analysis of the convergence behavior of HDMR expansion is not given in this paper, numerical tests

on a number of systems suggest that low-order terms will represent the output to good accuracy. The systems include chemical kinetics modelling [26], radiative transport modelling [27], solid-state material modelling and experiments [21,25], as well as testing on various simple mathematically defined tasks addressed in the text. We emphasize that HDMR is designed to deal with well-defined physical systems where the input variables are rationally chosen to have a nominally specific action or a role. The latter circumstance is natural in setting up physical systems, but no such guidance exists for arbitrary mathematical functions, notwithstanding the theorem by Kolmogorov. These comments are important to keep in mind when exploiting HDMRs.

Section 2 introduced the general formulation of HDMR and presented two particular HDMR expansions. The ANOVA-HDMR useful in statistics called for the computation of multi-dimensional integrals which is quite prohibitive in high dimensions at good accuracy. Although Monte-Carlo integration is viable in high dimensions, one still needs a large number of sample values to carry out the necessary integrations to good acuuracy. The cut-HDMR expansion does not necessitate the computation of any multi-dimensional integrals. It uses the sample values of the output on lines, planes and hyperplanes of higher dimensions passing through a reference point and constructs the function from these values according to equation (49). A very important result connecting the ANOVA-HDMR and cut-HDMR is that the ANOVA-HDMR approximation $f^{\text{anova}}(x)$ of the function $f(x)$ can be obtained in a much more efficient manner from $f^{\text{cut}}(x)$ taken to convergence. In this case, the ANOVA-HDMR of $f^{\text{cut}}(x)$ is a good approximation to $f^{\text{anova}}(x)$, and computing $f \rightarrow f^{\text{cut}} \rightarrow f^{\text{anova}}$ is often expected to be much less intensive for the same degree of accuracy compared to that of $f \rightarrow f^{\text{anova}}$, since the dimension of the integrals to be computed is smaller. Given the low dimension of the integrals, accurate quadrature techniques could be very efficient. In this case, the sampling of the cut-HDMR subspaces could be performed at the particular quadrature points. A graphical illustration of this method is given in figure 1.

New HDMR expansions with distinct character can be generated by changing the measure μ in formulae (16). The measure μ in this respect acts as a "weight" to give more importance to certain regions of the input space. Coordinate transformations of the original input variables also generate new HDMR expansions. Kolmogorov's theorem implies that there is a coordinate system in which the HDMR expansion is exact at first order. However, an *a priori* analysis of the output data must be performed first to learn which coordinate system is the best one. This task is as difficult as learning the output function and as an initial approximation one can search for optimal linear coordinate transformations which is the basis for the projection pursuit regression technique.

Section 3 extended the HDMR expansion to represent physical systems where inputs reside in an infinite-dimensional space, and thus the output becomes a functional. If a discretization of the input space is possible this functional becomes a function of the discretization coefficients, thus rendering a function HDMR expansion possible. However, a direct functional analog of HDMR can be expressed in terms of functional

integrals of the output functional. The interpretation of the component functionals is the same as in the function HDMR case. Monte-Carlo simulations may be used to compute the associated multi-dimensional functional integrals. Computations of these integrals are very costly and an additional complication is that the underlying measure on the input space may not be known. A functional cut-HDMR avoids computation of the integrals and uses a reference point in the input function space to construct an HDMR expansion based on the expressions in equation (75). Simple examples were given to illustrate the functional HDMR and functional cut-HDMR.

As a multivariate approximation/interpolation scheme, HDMR has a broad variety of applications. It can also be used in assessing the importance of the individual and cooperative effects of the input variables. Selected applications are mentioned in section 4. This list is not exhaustive and should be regarded as representative. The relative ease of employing HDMRs should aid in their various future applications.

Appendix

This appendix gives a brief primer on functional integration [6,29] and how to compute functional integrals by Monte-Carlo simulations. Functional HDMR is expressed in terms of integrals of output functionals with respect to a measure defined on the space of input functions. It is necessary to have a measure defined on the space of inputs to carry out the integration. For ease of understanding, the terminology of stochastic integration [16] will be used. The only difference with the general case is that the underlying measure is a probability measure. A stochastic process $\{X_t\}_{t\in T}$ is an indexed family of "random variables" defined on a probability space $(\Omega, \mathcal{F}, \mathbf{P})$ with Ω an abstract space, $\mathcal{F}$ a σ-algebra defined on Ω and $\mathbf{P}$ a probability measure defined on $\mathcal{F}$. The parameter space T is the unit interval $[0,1]$. Note that, for each $t \in T$ fixed, one has a random variable (a measurable function in the general case). On the other hand, fixing $\omega \in \Omega$ one can consider the function $t \to X_t(\omega)$, $t \in T$, which is called a *path* of X_t. One can identify each ω with the function $t \to X_t(\omega)$ from T into $\mathbf{R}^n$. Thus, we can regard Ω as a subset of the space $\overline{\Omega} = (\mathbf{R}^n)^T$ of all functions from T into $\mathbf{R}^n$. Then the σ-algebra $\mathcal{F}$ will contain the σ-algebra $\mathcal{B}$ generated by the sets of the form

$$\{\omega\colon\ \omega(t_1) \in F_1,\ \omega(t_2) \in F_2,\ \ldots,\ \omega(t_k) \in F_k\}, \quad F_i \subset \mathbf{R}^n \text{ Borel sets.} \tag{83}$$

Therefore, a stochastic process may be viewed as a probability measure $\mathbf{P}$ on the measurable space $((\mathbf{R}^n)^T, \mathcal{B})$.

The finite-dimensional distributions of the process $X \equiv \{X_t\}_{t\in T}$ are the measures $\mu_{t_1,t_2,\ldots,t_k}$ defined on $\mathbf{R}^{nk}$, $k = 1, 2, \ldots$, by

$$\mu_{t_1,t_2,\ldots,t_k}(F_1 \times F_2 \times \cdots \times F_k) = \mathbf{P}[X_{t_1} \in F_1,\ X_{t_2} \in F_2,\ \ldots,\ X_{t_k} \in F_k], \quad t_i \in T, \tag{84}$$

where F_i are Borel sets in $\mathbf{R}^n$. The family of finite distributions specifies the process X. Two stochastic process X_t and Y_t are modifications of each other if $\mathbf{P}[\omega\colon\ X_t(\omega) =$

$Y_t(\omega)] = 1$ for all $t \in T$. Kolmogorov's continuity theorem states that, if the stochastic process X satisfies the condition

$$\mathbf{E}\big[|X_t - X_s|^{\alpha}\big] \leqslant C|t-s|^{1+\beta}, \quad 0 \leqslant s,t \leqslant T, \tag{85}$$

for some positive constants α, β, C, then there exists a continuous modification of X. From here we deal with processes which have continuous modifications.

X is said to be a Gaussian process if the vector $(X_{t_1}, X_{t_2}, \ldots, X_{t_k})$ is Gaussian for every choice of the integer $n \geqslant 1$ and times $t_1, t_2, \ldots, t_k$. A *Wiener process* $\{W_t\}_{t\in T}$ is a continuous Gaussian process with mean zero and covariance function

$$\mathrm{Cov}(W_s, W_t) \equiv \mathbf{E}[W_s W_t] = \min(s,t). \tag{86}$$

An m-dimensional Wiener process is defined as a vector process

$$W \equiv \big[W_1(t), W_2(t), \ldots, W_m(t)\big], \tag{87}$$

where one-dimensional processes $\{W_i(t)\}_{t\geqslant 0}$ are independent one-dimensional Wiener processes. The *Wiener measure* μ^W generated by the Wiener process has the following finite-dimensional distributions. Fix $x \in \mathbf{R}^n$ and define

$$\begin{aligned} p(t,x) &\equiv (2\pi t)^{-n/2}\, \mathrm{e}^{-|x-y|^2/(2t)}, \quad t \in T, \\ \mu^W{}_{t_1,t_2,\ldots,t_k}(F_1 \times F_2 \times \cdots \times F_k) &\equiv \int_{F_1\times\cdots\times F_k} p(t_1,x,x_1)p(t_2-t_1,x_1,x_2)\times\cdots \\ &\quad \times p(t_k - t_{k-1}, x_{k-1}, x_k)\,\mathrm{d}x_1 \ldots \mathrm{d}x_k. \end{aligned} \tag{88}$$

If an integrable functional $F[W]$ is given, the Wiener integral is defined by

$$\int_C F[W]\,\mu^W(\mathrm{d}W) \equiv \mathbf{E}FW, \tag{89}$$

where $C = C^m[0,1]$ and the expectation is taken with respect to measure μ^W. For the class of functionals $F[W] = ||W||^{2k} = \int_0^1 W^{2k}(t)\,\mathrm{d}t$, the exact values of the integrals $c_k = \mathbf{E}FW$ are given by the following recursive formulae:

$$c_0 = 1, \qquad c_k = 2^k \frac{\mathrm{d}^k}{\mathrm{d}\lambda^k}\{\cos\lambda\}^{-1/2}|_{\lambda=0}. \tag{90}$$

The first few are

$$c_1 = \frac{1}{2}, \qquad c_2 = \frac{7}{12}, \qquad c_3 = \frac{139}{120}, \qquad c_4 = \frac{5473}{1680}. \tag{91}$$

The Monte-Carlo method of approximating integrable functionals is given in its simplest form by the formula

$$\int_C F[W]\,\mu^W(\mathrm{d}W) \equiv \mathbf{E}F[W] \approx \frac{1}{N}\sum_{k=1}^{N} F\big[W^{(k)}\big], \tag{92}$$

where $W^{(k)}$ are independent realizations of the m-dimensional Wiener process. As N grows, the quantity $(1/N)\sum_{k=1}^{N} F[W^{(k)}]$ converges in probability to the functional integral of FW with respect to the m-fold Wiener measure on the function space $C[0,1]^m$. The computation scheme above can also be used for the evaluation of functional integrals where the input functions are non-random. Then the convergence is in the ordinary sense, rather than a probabilistic one.

One approximate realization of a one-dimensional Wiener process is based on the substitution of the trajectories by polygonal lines. First, partition the segment $[0,1]$ into n parts by the points $0 = t_0 < t_1 < \cdots < t_n = 1$. By the definition of the Wiener process, the random values $W(t_i)$, $i = 1, 2, \ldots, n$, of the Brownian trajectory may be consecutively found from a known value $W(t_{i-1})$ ($W(0) = 0$) as the conditional normal distribution with parameters $m = W(t_{i-1})$ and $\sigma^2 = t_i - t_{i-1}$. Equivalently, the values $W(t_i)$ may be specified by the formula

$$W(t_i) = W(t_{i-1}) + \sqrt{t_i - t_{i-1}}\zeta_i \quad (i = 1, 2, \ldots, n), \tag{93}$$

where ζ_i are independent normal random values with parameters $m = 0$, $\sigma^2 = 1$. Thus, the realization $x_k(t)$, $k = 1, \ldots, N$, of Brownian motion $W(t)$ is by polygonal lines

$$W(t) = W(t_{i-1}) + \frac{W(t_i) - W(t_{i-1})}{t_i - t_{i-1}}(t - t_{i-1}) \quad \big(t \in [t_{i-1}, t_i]\big) \tag{94}$$

or, in a slightly different form,

$$W(t) = W(t_{i-1}) + \frac{t - t_{i-1}}{\sqrt{t_i - t_{i-1}}}\zeta_i \quad \big(t \in [t_{i-1}, t_i]\big),$$
$$W(0) = 0, \quad i = 1, 2, \ldots, n,$$

which may be constructed by modeling the above-mentioned random quantities ζ_i.

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