Ratio Control Variate Method for Efficiently Determining High-Dimensional Model Representations

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Abstract: The High-Dimensional Model Representation (HDMR) technique is a family of approaches to efficiently interpolate high-dimensional functions. RS(Random Sampling)-HDMR is a practical form of HDMR based on randomly sampling the overall function, and utilizing orthonormal polynomial expansions to approximate the RS-HDMR component functions. The determination of the expansion coefficients for the component functions employs Monte Carlo integration, which controls the accuracy of the RS-HDMR interpolation. The control variate method is an established approach to improve the accuracy of Monte Carlo integration. However, this method is often not practical for an arbitrary function $f(\mathbf{x})$ because there is no general way to find the analytical control variate function $h(\mathbf{x})$, which needs to be very similar to $f(\mathbf{x})$. In this article, we show that truncated RS-HDMR expansions can be used as $h(\mathbf{x})$ for arbitrary $f(\mathbf{x})$, and a more stable iterative ratio control variate method was developed for the determination of the expansion coefficients for the RS-HDMR component functions. As the asymptotic error (standard deviation) of the estimator given by the ratio control variate method is proportional to $1/N$(sample size), it is more efficient than the direct Monte Carlo integration, whose error is proportional to $1/\sqrt{N}$. In an illustration of a four-dimensional atmospheric model a few hundred random samples are sufficient to construct an RS-HDMR expansion by the ratio control variate method with an accuracy comparable to that obtained by direct Monte Carlo integration with thousands of samples.

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Introduction

The high-dimensional model representation (HDMR) technique is being developed for interpolation of high-dimensional input–output systems.[1–4] HDMR expresses the system output $f(\mathbf{x})$ as a finite hierarchical cooperative function expansion in terms of its input variables:

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1\le i<j\le n} f_{ij}(x_i, x_j) + \cdots + \sum_{1\le i_1<\cdots<i_l\le n} f_{i_1 i_2 \ldots i_l}(x_{i_1}, x_{i_2}, \ldots, x_{i_l}) + \cdots + f_{12\ldots n}(x_1, x_2, \ldots, x_n), \quad (1)$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_n)$; f_0, $f_i(x_i)$, $f_{ij}(x_i, x_j)\cdots$ are called zeroth; first; second; ... order component functions of HDMR, respectively.

Distinct, but formally equivalent HDMR expansions, all of the same structure as eq. (1), may be constructed. RS(Random Sampling)-HDMR is based on randomly sampling the overall function $f(\mathbf{x})$. For RS-HDMR, the variables x_i are first normalized by some suitable transformations such that $0 \le x_i \le 1$ for all i. The output function $f(\mathbf{x})$ is then defined in the unit hypercube $K^n = \{(x_1, x_2, \ldots, x_n) | 0 \le x_i \le 1, i = 1, 2, \ldots, n\}$. The independent random input variable $x_i (i = 1, 2, \ldots, n)$ has the probability density function $w_i(x_i)$ satisfying the conditions

$$\begin{cases} w_i(x_i) \ge 0, & (0 \le x_i \le 1), \\ \int_0^1 w_i(x_i) dx_i = 1, & (i = 1, 2, \ldots, n). \end{cases} \quad (2)$$

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The component functions of RS-HDMR have the following forms:[5]

$$f_0 = \int_{K^n} \prod_{i=1}^{n} w_i(x_i) f(\mathbf{x}) d\mathbf{x}, \tag{3}$$

$$f_i(x_i) = \int_{K^{n-1}} \prod_{\substack{k=1 \\ k\neq i}}^{n} w_k(x_k) f(\mathbf{x}) d\mathbf{x}^i - f_0, \tag{4}$$

$$f_{ij}(x_i, x_j) = \int_{K^{n-2}} \prod_{\substack{k=1 \\ k\neq i,j}}^{n} w_k(x_k) f(\mathbf{x}) d\mathbf{x}^{ij} - f_i(x_i) - f_j(x_j) - f_0, \tag{5}$$

$$\ldots,$$

where $d\mathbf{x}^i$ and $d\mathbf{x}^{ij}$ are just the product $dx_1 dx_2 \cdots dx_n$ without dx_i and $dx_i dx_j$, respectively. Finally, the last term $f_{12\ldots n}(x_1, x_2, \ldots, x_n)$ is determined from the difference between $f(\mathbf{x})$ and all the other component functions in eq. (1).

Practical approaches to determine the RS-HDMR component functions have been developed[5,6] based on approximating them with weighted orthonormal polynomials $\{\varphi\}$ as

$$f_i(x_i) \approx \sum_{r=1}^{k} \alpha_r^i \varphi_r^i(x_i), \tag{6}$$

$$f_{ij}(x_i, x_j) \approx \sum_{p=1}^{l} \sum_{q=1}^{l'} \beta_{pq}^{ij} \varphi_p^i(x_i) \varphi_q^j(x_j), \tag{7}$$

$$f_{ijk}(x_i, x_j, x_k) \approx \sum_{p=1}^{m} \sum_{q=1}^{m'} \sum_{r=1}^{m''} \gamma_{pqr}^{ijk} \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k), \tag{8}$$

$$\ldots,$$

where k, l, l', m, m', m'' are integers; $\alpha_r^i, \beta_{pq}^{ij}$ and γ_{pqr}^{ijk} are constant coefficients to be determined. The polynomials $\{\varphi\}$ possess the weighted orthonormality properties:

$$\int_0^1 w_i(x_i) \varphi_r^i(x_i) dx_i = 0, \quad \text{for all } r, i, \tag{9}$$

$$\int_0^1 w_i(x_i) \left[\varphi_r^i(x_i)\right]^2 dx_i = 1, \quad \text{for all } r, i, \tag{10}$$

$$\int_0^1 w_i(x_i) \varphi_p^i(x_i) \varphi_q^i(x_i) dx_i = 0, \quad p \neq q, \tag{11}$$

implying that they have a zero mean, unit norm, and are mutually orthogonal with respect to the weight $w_i(x_i)$. In most cases, using only $\varphi_1^i(x_i), \varphi_2^i(x_i)$ and $\varphi_3^i(x_i)$ (i.e., $k, l, l', m, m', m'' \leq 3$) often results in satisfactory accuracy.

When the Monte Carlo integration approximation is employed, eqs. (9)–(11) are equivalent to the approximations

$$\int_0^1 w_i(x_i) \varphi_r^i(x_i) dx_i \approx \frac{1}{N} \sum_{s=1}^{N} \varphi_r^i\left(x_i^{(s)}\right) = \xi_r^i \neq 0, \quad (r = 1, 2, \ldots) \tag{12}$$

$$\int_0^1 w_i(x_i) \left[\varphi_r^i(x_i)\right]^2 dx_i \approx \frac{1}{N} \sum_{s=1}^{N} \left[\varphi_r^i\left(x_i^{(s)}\right)\right]^2 = \zeta_r^i \neq 1, \quad (r = 1, 2, \ldots) \tag{13}$$

$$\int_0^1 w_i(x_i) \varphi_p^i(x_i) \varphi_q^i(x_i) dx_i \approx \frac{1}{N} \sum_{s=1}^{N} \varphi_p^i\left(x_i^{(s)}\right) \varphi_q^i\left(x_i^{(s)}\right) = \eta_{pq}^i \neq 0, \quad (p \neq q) \tag{14}$$

where ξ_r^i and η_{pq}^i are small numbers, but not exactly equal to zero, ζ_r^i are close to but not equal to unity; and, their values depend on the sample used. This implies that the weighted orthonormality property is not exactly fulfilled when the Monte Carlo integration approximation is employed. This may cause some additional error. To reduce this error, we define *optimal* weighted orthonormal polynomials for different samples as follows:[5]

$$\varphi_1^i(x_i) = a_1 x_i + a_0, \tag{15}$$

$$\varphi_2^i(x_i) = b_2 x_i^2 + b_1 x_i + b_0, \tag{16}$$

$$\varphi_3^i(x_i) = c_3 x_i^3 + c_2 x_i^2 + c_1 x_i + c_0, \tag{17}$$

$$\ldots\ldots$$

where the coefficients $a_0, a_1, b_0, \ldots, c_3$ are determined in such a way that for a given set of random samples (generated by $\{w_i(x_i)\}$) $\sum_r [(\xi_r^i)^2 + (\zeta_r^i - 1)^2] + \sum_{p<q} (\eta_{pq}^i)^2$ is minimized. This implies that the weighted orthonormality property is forced to be best satisfied for a given set of data. In our previous calculations for different systems and sample sizes, $\xi_r^i, 1 - \zeta_r^i$ and η_{pq}^i were smaller than 10^{-9}.

Optimal weighted orthonormal polynomials for variable x_i best satisfy the weighted orthonormality property, but the Monte Carlo integration approximation of the integrals for the products $\varphi_p^i(x_i)\varphi_q^j(x_j)(i \neq j)$ cannot guarantee the weighted orthonormality property between the basis functions with different variables. However, the weighted orthonormality property will be improved by increasing sample size N.

Using the optimal weighted orthonormal polynomial approximation, eq. (1) can be expressed as

$$f(\mathbf{x}) \approx f_0 + \sum_{i=1}^{n} \sum_{r=1}^{k} \alpha_r^i \varphi_r^i(x_i) + \sum_{1\leq i<j\leq n} \sum_{p=1}^{l} \sum_{q=1}^{l'} \beta_{pq}^{ij} \varphi_p^i(x_i) \varphi_q^j(x_j) + \sum_{1\leq i<j<k\leq n} \sum_{p=1}^{m} \sum_{q=1}^{m'} \sum_{r=1}^{m''} \gamma_{pqr}^{ijk} \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) + \cdots. \tag{18}$$

The coefficients $\{\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}\}$ can be determined by using the weighted orthonormality properties of $\{\varphi\}$, for example,

$$\alpha_r^i = \int_{K^n} \prod_{k=1}^{n} w_k(x_k) f(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x}. \tag{19}$$

The integral on the right-hand side of the above equation may be approximated by direct Monte Carlo integration so that

$$\alpha_r^i = \int_{K^n} \prod_{k=1}^{n} w_k(x_k) f(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x} \approx \frac{1}{N} \sum_{s=1}^{N} f(\mathbf{x}^{(s)}) \varphi_r^i\left(x_i^{(s)}\right), \tag{20}$$

where $\mathbf{x}^{(s)} = (x_1^{(s)}, x_2^{(s)}, \ldots, x_n^{(s)})(s = 1, 2, \ldots, N)$ is the sth random sample point, and N is the total number of random samples.

The standard deviation (or standard error) of this approximation is proportional to the standard deviation of the integrand $f(\mathbf{x})\varphi_r^i(x_i)$ divided by $\sqrt{N}$.[7]

Similarly, we have

$$\begin{aligned}\beta_{pq}^{ij} &= \int_{K^n} \prod_{k=1}^{n} w_k(x_k) f(\mathbf{x}) \varphi_p^i(x_i) \varphi_q^j(x_j) d\mathbf{x} \\ &\approx \frac{1}{N} \sum_{s=1}^{N} f\left(\mathbf{x}^{(s)}\right) \varphi_p^i\left(x_i^{(s)}\right) \varphi_q^j\left(x_j^{(s)}\right), \qquad (21)\\ \gamma_{pqr}^{ijk} &= \int_{K^n} \prod_{l=1}^{n} w_l(x_l) f(\mathbf{x}) \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) d\mathbf{x} \\ &\approx \frac{1}{N} \sum_{s=1}^{N} f\left(\mathbf{x}^{(s)}\right) \varphi_p^i\left(x_i^{(s)}\right) \varphi_q^j\left(x_j^{(s)}\right) \varphi_r^k\left(x_k^{(s)}\right), \qquad (22)\\ &\cdots.\end{aligned}$$

The formulas in eqs. (20)–(22) have the same form and automatically tailored to the particular probability distribution function when the sampling is drawn under the guidance by the weight $\{w_i(x_i)\}$.[5]

The error of the Monte Carlo integration can be reduced either by increasing the sample size N or decreasing the variance of the integrands in eqs. (20)–(22) upon the introduction of special techniques. Monte Carlo integration error becomes troublesome when random sampling of the integrand produces a large variance, that is, the integrand has rapid changes in the desired domain, especially in sign. This behavior is expected to arise when considering the integrands in eqs. (20)–(22) with large numbers of basis function products such as $f(\mathbf{x})\varphi_p^i(x_i)\varphi_q^j(x_j)$ and $f(\mathbf{x})\varphi_p^i(x_i)\varphi_q^j(x_j)\varphi_r^k(x_k)$. Therefore, the determination of the high-order RS-HDMR component functions generally requires additional samples. For example, to determine $f_i(x_i)$, a few hundred samples may give good accuracy, but for $f_{ij}(x_i, x_j)$ to achieve the same accuracy may require thousands of samples. For $f_{ijk}(x_i, x_j, x_k)$ even thousands of samples may not be sufficient. However, for practical reasons, the sample size is often restricted by time and cost considerations. Besides increasing N, the other way to improve the accuracy of the Monte Carlo integration is to reduce the variance of the integrand. This article exploits the control variate method[8] in RS-HDMR for this purpose. The previous correlation method[9] and the ratio control variate method belong to this category; it will be shown that the control variate method is generally superior in performance in the context of RS-HDMR.

The article is organized as follows. Section 2 introduces the control variate method of Monte Carlo integration in RS-HDMR, and Section 3 presents an illustration of this method for an atmospheric chemical kinetics model. Finally, Section 4 presents some concluding remarks.

Control Variate Methods for Variance Reduction of Monte Carlo Integration in RS-HDMR

Control variate methods are established approaches to improve the accuracy of Monte Carlo integration.[7,9] Consider an integral for the determination of any coefficient in eqs. (20)–(22), for example

$$\begin{aligned}\alpha_r^i &= \int_{K^n} \prod_{i=1}^{n} w_i(x_i) f(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x} \\ &\approx \frac{1}{N} \sum_{s=1}^{N} f\left(\mathbf{x}^{(s)}\right) \varphi_r^i\left(x_i^{(s)}\right).\end{aligned}$$

To reduce the variance of the integrand $f(\mathbf{x})\varphi_r^i(x_i)$ in K^n, we seek a control variate $h(\mathbf{x})$ satisfying two conditions: (1) $f(\mathbf{x})$ and $h(\mathbf{x})$ are very similar over the entire domain of $\mathbf{x}$; (2) the integral $\int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x}$ can be obtained analytically.

Additive Control Variate—the Correlation Method

One way to use the control variate technique is to rewrite eq. (20) as

$$\begin{aligned}\alpha_r^i = &\int_{K^n} \prod_{i=1}^{n} w_i(x_i) [f(\mathbf{x}) - h(\mathbf{x})] \varphi_r^i(x_i) d\mathbf{x} \\ &+ \int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x}. \qquad (23)\end{aligned}$$

The first term in eq. (23) has a small variance when $h(\mathbf{x})$ and $f(\mathbf{x})$ have a strong linear relationship (i.e., $h(\mathbf{x}) \approx f(\mathbf{x}) + b$ with b being a constant). Because the second integral is known analytically as

$$\int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x} = c_r^i, \qquad (24)$$

the variance comes only from the first term in eq. (23). As $f(\mathbf{x}) - h(\mathbf{x})$ is almost constant or zero everywhere by assumption, we expect that

$$\operatorname{var}\left\{\prod_{i=1}^{n} w_i(x_i) [f(\mathbf{x}) - h(\mathbf{x})] \varphi_r^i(x_i)\right\} < \operatorname{var}\left\{\prod_{i=1}^{n} w_i(x_i) f(\mathbf{x}) \varphi_r^i(x_i)\right\}, \qquad (25)$$

and α_r^i may be obtained by approximating the first integral in eq. (23) with Monte Carlo integration

$$\alpha_r^i \approx \frac{1}{N} \sum_{s=1}^{N} \left[f\left(\mathbf{x}^{(s)}\right) - h\left(\mathbf{x}^{(s)}\right)\right] \varphi_r^i\left(x_i^{(s)}\right) + c_r^i \qquad (26)$$

to have better accuracy than that given by eq. (20). However, this additive control variate method is often not practical for an arbitrary function $f(\mathbf{x})$ because there is no general way to find the analytical control variate function $h(\mathbf{x})$. The task of finding $h(\mathbf{x})$ becomes even more difficult when the analytic form of $f(\mathbf{x})$ is not known, but only some values of $f(\mathbf{x})$ can be sampled.

Fortunately, a truncated RS-HDMR expansion of eq. (18) satisfies these requirements and can be used as $h(\mathbf{x})$, for instance

$$\begin{aligned}h(\mathbf{x}) = f_0 &+ \sum_{i=1}^{n} \sum_{r=1}^{k} \bar{\alpha}_r^i \varphi_r^i(x_i) + \sum_{1 \le i < j \le n} \sum_{p=1}^{l} \sum_{q=1}^{l'} \bar{\beta}_{pq}^{ij} \varphi_p^i(x_i) \varphi_q^j(x_j) \\ &+ \sum_{1 \le i < j < k \le n} \sum_{p=1}^{m} \sum_{q=1}^{m'} \sum_{r=1}^{m''} \bar{\gamma}_{pqr}^{ijk} \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k), \qquad (27)\end{aligned}$$

where the coefficients $\{\bar{\alpha}_r^i, \bar{\beta}_{pq}^{ij}, \bar{\gamma}_{pqr}^{ijk}\}$ are determined by direct Monte Carlo integration given in eqs. (20)–(22). The difference $f(\mathbf{x}) - h(\mathbf{x})$ should be small if the truncated RS-HDMR expansion is a good approximation of $f(\mathbf{x})$. The integration of $h(\mathbf{x})$ with respect to $\mathbf{x}$ can be obtained analytically using the orthonormality property of $\{\varphi\}$

$$\int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x} = \int_{K^n} \prod_{i=1}^{n} w_i(x_i) \Bigg[f_0 + \sum_{i=1}^{n} \sum_{r'=1}^{k} \bar{\alpha}_{r'}^i \varphi_{r'}^i(x_i) + \sum_{1\le i<j\le n} \sum_{p=1}^{l} \sum_{q=1}^{l'} \bar{\beta}_{pq}^{ij} \varphi_p^i(x_i) \varphi_q^j(x_j) + \sum_{1\le i<j<k\le n} \sum_{p=1}^{m} \sum_{q=1}^{m'} \sum_{r'=1}^{m''} \bar{\gamma}_{pqr}^{ijk} \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_{r'}^k(x_k) \Bigg] \varphi_r^i(x_i) d\mathbf{x} = \bar{\alpha}_r^i, \tag{28}$$

and then

$$\alpha_r^i \approx \frac{1}{N} \sum_{s=1}^{N} \left[f\left(\mathbf{x}^{(s)}\right) - h\left(\mathbf{x}^{(s)}\right) \right] \varphi_r^i\left(x_i^{(s)}\right) + \bar{\alpha}_r^i. \tag{29}$$

Similarly, we also have

$$\beta_{pq}^{ij} \approx \frac{1}{N} \sum_{s=1}^{N} \left[f\left(\mathbf{x}^{(s)}\right) - h\left(\mathbf{x}^{(s)}\right) \right] \varphi_p^i\left(x_i^{(s)}\right) \varphi_q^j\left(x_j^{(s)}\right) + \bar{\beta}_{pq}^{ij}, \tag{30}$$

$$\gamma_{pqr}^{ijk} \approx \frac{1}{N} \sum_{s=1}^{N} \left[f\left(\mathbf{x}^{(s)}\right) - h\left(\mathbf{x}^{(s)}\right) \right] \varphi_p^i\left(x_i^{(s)}\right) \varphi_q^j\left(x_j^{(s)}\right) \varphi_r^k\left(x_k^{(s)}\right) + \bar{\gamma}_{pqr}^{ijk}. \tag{31}$$

Equations (29)–(31) show that the first terms in these equations are corrections for the initial values $\bar{\alpha}_r^i$, $\bar{\beta}_{pq}^{ij}$ and $\bar{\gamma}_{pqr}^{ijk}$. The resultant α_r^i, β_{pq}^{ij} and γ_{pqr}^{ijk} may be reused as initial values for the construction of a new $h(\mathbf{x})$ with a even smaller variance for $f(\mathbf{x}) - h(\mathbf{x})$ to repeat the calculation again. Then, eqs. (29)–(31) become an iteration procedure for a given set of random samples. When $h(\mathbf{x})$ is exactly equal to $f(\mathbf{x})$, the first term in eqs. (29)–(31) vanishes. In practice, $h(\mathbf{x})$ is only a good approximation of $f(\mathbf{x})$, and the first term in eqs. (29)–(31) for the given samples never vanishes in the iteration, but it can be very small and oscillate around zero. Thus, a tolerance can be set. The iteration is terminated when the difference of two adjacent iterative values for a parameter is smaller than the given tolerance. The satisfaction of the tolerance criterion can be achieved if the initial $h(\mathbf{x})$ is close to $f(\mathbf{x})$ and the sample size N is large enough.

Notice that $\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}$ are all coupled in the operations above because they are all contained in $h(\mathbf{x})$. When $h(\mathbf{x})$ is the third-order expansion in eq. (27), the iteration may diverge for a small sample size. In this case we may choose the second-order expansion

$$h(\mathbf{x}) = f_0 + \sum_{i=1}^{n} \sum_{r=1}^{k} \bar{\alpha}_r^i \varphi_r^i(x_i) + \sum_{1\le i<j\le n} \sum_{p=1}^{l} \sum_{q=1}^{l'} \bar{\beta}_{pq}^{ij} \varphi_p^i(x_i) \varphi_q^j(x_j) \tag{32}$$

as the control variate. The coefficients α_r^i and β_{pq}^{ij} can be determined by iteration with eqs. (29) and (30). The resultant values of α_r^i and β_{pq}^{ij} are used to determine the coefficients γ_{pqr}^{ijk} by the following equation without iteration

$$\gamma_{pqr}^{ijk} \approx \frac{1}{N} \sum_{s=1}^{N} \left[f\left(\mathbf{x}^{(s)}\right) - h\left(\mathbf{x}^{(s)}\right) \right] \varphi_p^i\left(x_i^{(s)}\right) \varphi_q^j\left(x_j^{(s)}\right) \varphi_r\left(x_k^{(s)}\right) \tag{33}$$

because

$$\bar{\gamma}_{pqr}^{ijk} = \int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) d\mathbf{x} = \int_{K^n} \prod_{i=1}^{n} w_i(x_i) \Bigg[f_0 + \sum_{i=1}^{n} \sum_{r'=1}^{k} \bar{\alpha}_{r'}^i \varphi_{r'}^i(x_i) + \sum_{1\le i<j\le n} \sum_{p'=1}^{l} \sum_{q'=1}^{l'} \bar{\beta}_{p'q'}^{ij} \varphi_{p'}^i(x_i) \varphi_{q'}^j(x_j) \Bigg] \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) d\mathbf{x} = 0. \tag{34}$$

This is the correlation method developed previously.[9]

The condition for the convergence of the iteration given by eqs. (29)–(31) is discussed below. Let

$$\mathbf{y}_0 = \left(\bar{\alpha}_1^1, \bar{\alpha}_2^1, \ldots, \bar{\beta}_{11}^{12}, \bar{\beta}_{12}^{12}, \ldots, \bar{\gamma}_{111}^{123}, \bar{\gamma}_{112}^{123}, \ldots, \bar{\gamma}_{mm'm''}^{(n-2)(n-1)n}\right)^T \tag{35}$$

be the initial values of all the constant parameters obtained by direct Monte Carlo integration, and

$$\mathbf{y}_k = \left(\alpha_1^1, \alpha_2^1, \ldots, \beta_{11}^{12}, \beta_{12}^{12}, \ldots, \gamma_{111}^{123}, \gamma_{112}^{123}, \ldots, \gamma_{mm'm''}^{(n-2)(n-1)n}\right)^T \tag{36}$$

be the resultant parameters in the kth iteration;

$$\mathbf{b} = \frac{1}{N} \sum_{s=1}^{N} f\left(\mathbf{x}^{(s)}\right) \left[\varphi_1^1\left(x_1^{(s)}\right), \varphi_2^1\left(x_1^{(s)}\right), \ldots, \varphi_1^1\left(x_1^{(s)}\right) \varphi_2^1\left(x_1^{(s)}\right), \ldots\right]^T, \tag{37}$$

$$A = \frac{1}{N} \sum_{s=1}^{N} \begin{bmatrix} \left[\varphi_1^1(x_1^{(s)})\right]^2 & \varphi_1^1\left(x_1^{(s)}\right) \varphi_2^1\left(x_1^{(s)}\right) & \cdots & \varphi_1^1\left(x_1^{(s)}\right) \varphi_m^{n-2}\left(x_{n-2}^{(s)}\right) \varphi_{m'}^{n-1}\left(x_{n-1}^{(s)}\right) \varphi_{m''}^n\left(x_n^{(s)}\right) \\ \varphi_2^1\left(x_1^{(s)}\right) \varphi_1^1\left(x_1^{(s)}\right) & \left[\varphi_2^1(x_1^{(s)})\right]^2 & \cdots & \varphi_2^1\left(x_1^{(s)}\right) \varphi_m^{n-2}\left(x_{n-2}^{(s)}\right) \varphi_{m'}^{n-1}\left(x_{n-1}^{(s)}\right) \varphi_{m''}^n\left(x_n^{(s)}\right) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_m^{n-2}\left(x_{n-2}^{(s)}\right) \varphi_{m'}^{n-1}\left(x_{n-1}^{(s)}\right) \varphi_{m''}^n\left(x_n^{(s)}\right) \varphi_1^1\left(x_1^{(s)}\right) & \cdots & \cdots & \left[\varphi_m^{n-2}(x_{n-2}^{(s)}) \varphi_{m'}^{n-1}(x_{n-1}^{(s)}) \varphi_{m''}^n(x_n^{(s)})\right]^2 \end{bmatrix}. \tag{38}$$

It is easy to prove that eqs. (29)–(31) can be represented in matrix form

$$\mathbf{y}_1 = \mathbf{b} + (I - A)\mathbf{y}_0, \tag{39}$$

and

$$\mathbf{y}_k = [I + (I - A) + \cdots + (I - A)^{k-1}]\mathbf{b} + (I - A)^k \mathbf{y}_0, \tag{40}$$

$$\mathbf{y}_n - \mathbf{y}_{n-1} = (I - A)^{n-1}(\mathbf{b} - A\mathbf{y}_0), \tag{41}$$

where I is the n-dimensional identity matrix. The iteration is convergent if and only if the norm $\|\mathbf{y}_n - \mathbf{y}_{n-1}\|$ approaches zero when $n \to \infty$. Because

$$\|\mathbf{y}_n - \mathbf{y}_{n-1}\| \le \|(I - A)\|^{n-1}\|\mathbf{b} - A\mathbf{y}_0\|, \tag{42}$$

and $\|\mathbf{b} - A\mathbf{y}_0\|$ is constant, the necessary and sufficient condition for iteration convergence is

$$\|(I - A)\| < 1. \tag{43}$$

When optimal weighted orthonormal polynomials $\varphi_r^i(x_i)$ are used,[5] the diagonal elements of A are very close to unity, and off-diagonal elements are small and close to zero. Consequently, all the elements of $I - A$ are small, and closer to zero when N becomes larger. If the norm $\|I - A\|_\infty$ is used, that is,

$$\|I - A\|_\infty = \max\left(\sum_{j=1}^{l} |(I - A)_{ij}|, \quad i = 1, 2, \ldots, l\right), \tag{44}$$

where $(I - A)_{ij}$ is the (i, j)-entry of $I - A$, and l is the dimension of A (i.e., the total number of the terms in eq. (27)). The value of $\|I - A\|_\infty$ depends on l and N. When N is large enough, $\|I - A\|_\infty < 1$ can be guaranteed.

Ratio Control Variate Method

Another way to use the control variate technique is to rewrite eq. (20) as

$$\alpha_r^i = \int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x} \frac{\int_{K^n} \prod_{i=1}^{n} w_i(x_i) f(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x}}{\int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x}}, \tag{45}$$

where $\int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_r^i(x_i) d\mathbf{x} \neq 0$. The first term in eq. (45) can be obtained analytically, and the second term has a small variance when $h(\mathbf{x})$ is almost equal to or proportional to $f(\mathbf{x})$ (i.e., $h(\mathbf{x}) \approx bf(\mathbf{x})$ with b being a constant). Then the second term in eq. (45) can be approximated well by Monte Carlo integration. Thus, we have

$$\alpha_r^i \approx \bar{\alpha}_r^i \frac{\sum_{s=1}^{N} f(\mathbf{x}^{(s)}) \varphi_r^i(x_i^{(s)})}{\sum_{s=1}^{N} h(\mathbf{x}^{(s)}) \varphi_r^i(x_i^{(s)})}. \tag{46}$$

Similarly, we also have

$$\beta_{pq}^{ij} \approx \bar{\beta}_{pq}^{ij} \frac{\sum_{s=1}^{N} f(\mathbf{x}^{(s)}) \varphi_p^i(x_i^{(s)}) \varphi_q^j(x_j^{(s)})}{\sum_{s=1}^{N} h(\mathbf{x}^{(s)}) \varphi_p^i(x_i^{(s)}) \varphi_q^j(x_j^{(s)})}, \tag{47}$$

$$\gamma_{pqr}^{ijk} \approx \bar{\gamma}_{pqr}^{ijk} \frac{\sum_{s=1}^{N} f(\mathbf{x}^{(s)}) \varphi_p^i(x_i^{(s)}) \varphi_q^j(x_j^{(s)}) \varphi_r^k(x_k^{(s)})}{\sum_{s=1}^{N} h(\mathbf{x}^{(s)}) \varphi_p^i(x_i^{(s)}) \varphi_q^j(x_j^{(s)}) \varphi_r^k(x_k^{(s)})}, \tag{48}$$

when the third-order expansion given in eq. (18) is used as the control variate. Similar to eqs. (29)–(31), eqs. (46)–(48) can be used to determine the coefficients $\{\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}\}$ iteratively, and the initial values $\{\bar{\alpha}_r^i, \bar{\beta}_{pq}^{ij}, \bar{\gamma}_{pqr}^{ijk}\}$ are given by direct Monte Carlo integration. When $h(\mathbf{x})$ is exactly equal to $f(\mathbf{x})$, the ratio in the second term in eqs. (46)–(48) is unity. In practice, the ratio in the second term in eqs. (47)–(48) for the given samples in the iteration will likely be close to unity. Similar to the correlation method, a tolerance can be set. The iteration is terminated when the difference of two adjacent iterative values for a parameter is smaller than the given tolerance. The satisfaction of the tolerance criterion can be achieved if the initial $h(\mathbf{x})$ is close to $f(\mathbf{x})$ and the sample size N is large enough.

When the second-order expansion in eq. (32) is used as the control variate, γ_{pqr}^{ijk} cannot be determined by eq. (48) because $\int_{K^n} \prod_{i=1}^{n} w_i(x_i) h(\mathbf{x}) \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) d\mathbf{x} = 0$. In this case, we write

$$\gamma_{pqr}^{ijk} = \int_{K^n} \prod_{i=1}^{n} w_i(x_i) g(\mathbf{x}) \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) d\mathbf{x} \times \frac{\int_{K^n} \prod_{i=1}^{n} w_i(x_i) [f(\mathbf{x}) - h(\mathbf{x})] \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) d\mathbf{x}}{\int_{K^n} \prod_{i=1}^{n} w_i(x_i) g(\mathbf{x}) \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k) d\mathbf{x}}, \tag{49}$$

where

$$g(\mathbf{x}) = \sum_{p=1}^{m} \sum_{q=1}^{m'} \sum_{r=1}^{m''} \bar{\gamma}_{pqr}^{ijk} \varphi_p^i(x_i) \varphi_q^j(x_j) \varphi_r^k(x_k). \tag{50}$$

When $f(\mathbf{x})$ can be accurately represented by the third-order expansion given in eq. (18), $f(\mathbf{x}) - h(\mathbf{x})$ can be well approximated by $g(\mathbf{x})$. The first term in eq. (49) can be obtained analytically as $\bar{\gamma}_{pqr}^{ijk}$, while the second term has a small variance and can be approximated by Monte Carlo integration, which gives

$$\gamma_{pqr}^{ijk} \approx \bar{\gamma}_{pqr}^{ijk} \frac{\sum_{s=1}^{N} [f(\mathbf{x}^{(s)}) - h(\mathbf{x}^{(s)})] \varphi_p^i(x_i^{(s)}) \varphi_q^j(x_j^{(s)}) \varphi_r^k(x_k^{(s)})}{\sum_{s=1}^{N} g(\mathbf{x}^{(s)}) \varphi_p^i(x_i^{(s)}) \varphi_q^j(x_j^{(s)}) \varphi_r^k(x_k^{(s)})}. \tag{51}$$

Table 1. The Relative Errors of the Different Order RS-HDMR Expansions for the Outputs $P, D, P - D$ Determined by Direct Monte Carlo Integration.

Sample size (N)	Relative error (%)	Data portion (%)[a]								
		P			D			$P - D$		
		1st	2nd	3rd	1st	2nd	3rd	1st	2nd	3rd
300	5	48.8	23.3	15.9	33.7	24.2	14.6	47.3	26.0	18.8
	10	69.3	44.2	30.7	55.0	43.4	28.1	72.5	51.8	36.1
	20	81.7	71.2	53.3	70.0	68.5	49.7	87.3	83.9	62.1
500	5	45.8	57.1	26.5	37.0	34.6	19.3	48.8	58.5	29.6
	10	68.6	78.3	47.1	55.7	59.6	36.8	72.2	83.4	52.3
	20	81.6	91.7	70.2	69.2	80.2	61.8	86.5	96.0	76.1
1000	5	46.3	72.6	48.6	38.6	58.6	36.8	49.6	77.5	50.7
	10	68.7	88.3	72.2	56.7	81.4	61.6	71.4	93.4	76.6
	20	81.8	96.6	88.5	69.7	93.6	83.8	86.4	99.3	92.8
3000	5	46.0	85.9	68.3	38.4	86.4	65.5	48.6	90.7	80.3
	10	68.5	95.7	88.7	55.4	95.5	84.0	70.9	97.7	94.2
	20	81.7	99.1	96.9	68.8	99.2	95.3	86.2	99.7	98.8
5000	5	45.7	90.4	85.7	38.4	91.8	75.9	48.5	93.8	90.4
	10	68.1	96.8	95.3	55.7	97.6	90.6	70.8	98.7	97.9
	20	81.6	99.4	98.9	68.9	99.6	97.1	86.2	99.9	99.8

[a]The percentage of 53,312 data with a relative error not larger than a given value.

Using eqs. (46)–(47) the coefficients $\alpha_r^i, \beta_{pq}^{ij}$ are determined iteratively first. Then using the resultant values of α_r^i and β_{pq}^{ij}, the coefficients γ_{pqr}^{ijk} may be determined by iteration with eq. (51). Similarly, the initial values $\{\bar{\alpha}_r^i, \bar{\beta}_{pq}^{ij}, \bar{\gamma}_{pqr}^{ijk}\}$ are given by direct Monte Carlo integration. As the asymptotic error of the estimator given by the ratio control variate method is proportional to $1/N$, while the error of the direct Monte Carlo integration is proportional to $1/\sqrt{N}$,[9] a few hundred random samples can be sufficient to determine the coefficients $\{\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}\}$ by the ratio control variate method with an accuracy comparable to that obtained by direct Monte Carlo integration with thousands of samples.

Illustration: A Photochemical Box Model

The same model used previously to test the correlation method is used again for the ratio control variate method. The model is a photochemical box model designed to treat the ozone chemistry in the background troposphere for studying three-dimensional global chemical transport.[10] This box model consists of 63 reactions and 28 chemical species used to calculate the rates of ozone production P, destruction D, and the tendency $P - D$ for incorporation into the overall three-dimensional model. The input random variables $\mathbf{x} = \{x_1, x_2, x_3, x_4\}$ are the concentrations of the four precursors: H_2O, CO, NO_x, and O_3. Five thousand random samples of $\mathbf{x}$ with a uniform distribution, that is, all $w_i(x_i) = 1$ were generated, and then the corresponding values for P, D, and $P - D$ were calculated by the model. The first to third-order orthonormal polynomials given in eqs. (12)–(14) were used to approximate the RS-HDMR component functions. For purposes of comparison, the expansion coefficients $\{\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}\}$ were determined by (1) direct Monte Carlo integration, (2) the correlation method, and (3) the ratio control variate method with different random sample sizes (300, 500, 1000, 3000, and 5000). The accuracy of the resultant different order RS-HDMR expansions were examined by comparison with 53,312 exact data, which uniformly cover the whole domain of $\mathbf{x}$. Table 1 gives the accuracy of different order RS-HDMR expansions for the three outputs whose component functions were approximated by third-order orthonormal polynomial expansions and $\{\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}\}$ were determined by direct Monte Carlo integration.

Table 1 shows that the sample size does not have a significant influence on the accuracy of the first-order RS-HDMR expansion, which means that α_r^i can be accurately determined with a few hundred samples. However, the sample size does have a significant influence on the accuracy of the second-order RS-HDMR expansion, and the determination of β_{pq}^{ij} may need thousands of samples. The third-order RS-HDMR expansion is worse than the second-order, and even the first-order RS-HDMR expansions when the sample size is small. Therefore, if several thousand samples are used, direct Monte Carlo integration may still be inaccurate for the determination of γ_{pqr}^{ijk}.

The ratio control variate method with Monte Carlo integration given by eqs. (46)–(48) was used to determine the coefficients $\alpha_r^i, \beta_{pq}^{ij}$ and γ_{pqr}^{ijk}. First, the third-order RS-HDMR given by eq. (27) with $k, l, l', m, m', m'' = 3$ was used as $h(\mathbf{x})$. Successful termination of the iteration was achieved with all sample sizes for $\alpha_r^i, \beta_{pq}^{ij}$, and γ_{pqr}^{ijk}, as in the final iterations the accuracy of the third-order RS-HDMR approximations remained almost constant. In contrast, the correlation method diverged when $N \leq 1000$. The results are given in Table 2, which shows that the ratio control variate method is a practical approach, which significantly reduces the variance, and hence improves the accuracy even for small sample sizes.

Table 2. The Relative Errors of the Resultant Third-Order RS-HDMR Expansions Determined by the Ratio Control Variate (I) and Correlation (II) Methods with Monte Carlo Integration Using the Third-Order RS-HDMR Expansion Given by eq. (27) as $h(\mathbf{x})$.

		Data portion (%)[a,b]					
Sample size (N)	Relative error (%)	P		D		$P-D$	
		I	II	I	II	I	II
300	5	93.5	—	84.2	—	91.1	—
	10	98.0	—	95.1	—	97.9	—
	20	99.6	—	98.8	—	99.8	—
500	5	87.7	—	93.5	—	99.8	—
	10	96.3	—	98.0	—	100	—
	20	99.4	—	99.6	—	100	—
1000	5	99.1	—	90.5	—	99.1	—
	10	99.8	—	96.3	—	99.9	—
	20	100	—	99.4	—	100	—
3000	5	98.8	99.9	98.3	99.7	99.1	99.7
	10	99.8	100	99.9	100	99.9	100
	20	100	100	100	100	100	100
5000	5	99.6	98.0	99.4	98.0	99.8	99.4
	10	99.9	99.4	99.9	99.5	99.9	99.9
	20	100	99.8	100	99.9	100	100

[a]The percentage of 53,312 data with a relative error not larger than a given value.
[b]Lack of convergence for the correlation method is donated by —.

Table 3. The Relative Errors of the Resultant Third-Order RS-HDMR Expansions Determined by Ratio Control Variate (I) and Correlation (II) Methods with Monte Carlo Integration Using the Second-Order RS-HDMR Expansion Given by eq. (32) as $h(\mathbf{x})$.

		Data portion (%)[a]					
Sample size (N)	Relative error (%)	P		D		$P-D$	
		I	II	I	II	I	II
300	5	91.3	93.6	77.8	92.7	96.8	98.9
	10	97.1	97.2	94.1	98.4	99.9	99.8
	20	99.2	99.6	98.8	100	100	100
500	5	94.2	95.6	94.6	96.5	96.6	98.0
	10	99.0	98.7	99.1	99.6	99.8	99.4
	20	99.9	99.8	100	100	100	99.8
1000	5	98.0	97.3	93.6	97.9	99.2	99.1
	10	99.5	99.1	98.1	99.7	99.9	99.7
	20	99.9	99.8	99.9	100	100	100
3000	5	98.7	99.2	98.0	99.6	99.7	99.5
	10	99.9	99.9	100	100	99.9	99.9
	20	100	100	100	100	100	100
5000	5	99.6	99.6	99.6	99.9	99.1	99.7
	10	100	100	100	100	99.9	100
	20	100	100	100	100	100	100

[a]The percentage of 53,312 data with a relative error not larger than a given value.

Table 3 gives the results from the second order expansion in eq. (32) as the control variate $h(\mathbf{x})$ using eqs. (46) and (47) and eq. (51) to determine the coefficients $\{\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}\}$. The results are satisfactory and comparable for both the ratio control variate and correlation methods. The ratio control variate method is a little worse for output D. The advantage of the ratio control variate method is that the second- and third-order RS-HDMR expansions can all be used as the control variate $h(\mathbf{x})$ to accurately determine all the coefficients $\{\alpha_r^i, \beta_{pq}^{ij}, \gamma_{pqr}^{ijk}\}$ with small sample sizes. Because only one set of random samples is needed, it is possible to construct truncated high-order RS-HDMR expansions from small random samples. This behavior is very attractive for interpolating high-dimensional systems, especially for cases where large data sets cannot be obtained easily.

Conclusions

This article showed that a truncated RS-HDMR expansion can act as a ratio control variate to very efficiently determine the RS-HDMR component functions. The ratio control variate method is more stable under iteration than the correlation method. An illustration showed that both the second- and third-order truncated RS-HDMR expansions can be used as the control variate. Because the asymptotic error of the ratio control variate method for Monte Carlo integration is proportional to the reciprocal of sample size, the resultant RS-HDMR approximation can produce satisfactory interpolative accuracy even for a few hundred samples, which is comparable to that obtained by direct Monte Carlo integration with thousands of samples.

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