Analyzing convergence criteria for Gerstner-Griebel and Ayres-Eaton

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1 Notation

- ξ - The vector of input variables $\xi = (\xi_1, \xi_2, \cdots, \xi_N)$
- Ω - The input space spanned by the input variable distributions
- g_k - The error between an iteration Λ_2 and Λ_1
- k - A combination of polynomial orders, given as a tuple
- Λ_1 - The set of all desired polynomial combinations k for the current iteration
- Λ_2 - The set of all desired polynomial combinations k for the next iteration
- $c_{i,k}$ - The scalar coefficient for polynomial combination with orders k in index set Λ_i
- Φ_k - The multidimensional orthonormal polynomial basis with degrees k.

2 Gerstner-Griebel

$$g_k = \max\left\{\alpha\frac{|\Delta_k f|}{|\Delta_1 f|}, \alpha\frac{n_1}{n_k}\right\}, \tag{1}$$

where n_k is the number of quadrature points with index set Λ_k, $\alpha \in [0.1]$ is a work scaling factor, and

$$\Delta_k f = (Q_k - Q_{k-1})f, \tag{2}$$

$$Q_k f = \sum_\ell w_\ell f(\xi_\ell), \tag{3}$$

which is an approximation as

$$\int_\Omega f(\xi)P(\xi)d\xi \approx \sum_\ell w_\ell f(\xi_\ell). \tag{4}$$

Thus, $|\Delta_k f|$ indicates the change in fidelity between one higher-order sparse quadrature set and a lower one. We desire to understand the numerical difference between successive quadratures. We consider the first moment of the function in probability space,

$$\mathbb{E}[f(\xi)] = \int_\Omega f(\xi)P(\xi)d\xi. \tag{5}$$

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With appropriate change of variable, we can rewrite the probability weighting term,

$$\mathbb{E}[f(\xi)] = \mathbb{E}[f(u)] = \int_\Omega f(u)du. \tag{6}$$

We now note that the function $f(u)$ can be expressed exactly as an infinite sum of orthogonal multidimensional polynomials $\Phi(u)$, as

$$f(u) = \sum_{i=0}^{\infty} f_{k_i}\Phi_{k_i}(u), \tag{7}$$

where $k \in \Lambda_\infty$ is a choice of polynomial order from Λ_∞ which contains all possible polynomials of any order spanned by the set of polynomials $\Phi(u)$, and f_{k_i} is a scaling coefficient for the i-th polynomial (which polynomial has multi-order k).

We consider $\Lambda_k \subset \Lambda_\infty$, which is a sparse index set that generates a sparse grid quadrature Q_k with points x_ℓ and weights w_ℓ, as

$$\int_\Omega g(x)dx \approx Q_k g(x) = \sum_{\ell=1}^{L} w_\ell g(x_\ell), \tag{8}$$

where $L = |Q_k|$ is the number of point-weight combinations in the sparse grid quadrature. $Q_k g(x)$ is exactly $\int g(x)dx$ only if $g(x)$ is a polynomial of order $J \equiv 2L-1$ (for Gauss quadrature). Returning to the first moment,

$$\mathbb{E}[f(u)] = \int_\Omega f(u)du, \tag{9}$$

we expand $f(u)$ using the orthogonal multidimensional polynomials,

$$\mathbb{E}[f(u)] = \int_\Omega \sum_{i=0}^{\infty} f_{k_i}\Phi_{k_i}(u)du. \tag{10}$$

We can then split the sum at an integration order J corresponding to a particular index set Λ_k,

$$\mathbb{E}[f(u)] = \int_\Omega \left[\sum_{i=0}^{J} f_{k_i}\Phi_{k_i}(u) + \sum_{i=J+1}^{\infty} f_{\tilde{k}_i}\Phi_{\tilde{k}_i}(u)\right] du, \tag{11}$$

where $\tilde{k} \in \Lambda_\infty$ while $k \in \Lambda_k$. In other words, $f(u)$ is split into two parts: that which is integrated exactly by the sparse grid quadrature Q_k generated by the index set Λ_k; and that which requires polynomials and coefficients not provided by the index set Λ_k but exists in Λ_∞. We rewrite and consider both terms independently.

$$\mathbb{E}[f(u)] = \int_\Omega \sum_{i=0}^{J} f_{k_i}\Phi_{k_i}(u)du + \int_\Omega \sum_{i=J+1}^{\infty} f_{\tilde{k}_i}\Phi_{\tilde{k}_i}(u)du. \tag{12}$$

The first term by definition is exactly integrated by the sparse quadrature Q_k,

$$\int_\Omega \sum_{i=0}^{J} f_{k_i}\Phi_{k_i}(u)du = \sum_{\ell=0}^{L} w_\ell \sum_{i=0}^{J} f_{k_i}\Phi_{k_i}(u_\ell) \tag{13}$$

$$= Q_k\left[\sum_{i=0}^{J} f_{k_i}\Phi_{k_i}(u)\right]. \tag{14}$$

Because of orthogonality and the nature of the polynomials over their domain, this simplifies to

$$Q_k \left[\sum_{i=0}^{J} f_{k_i} \Phi_{k_i}(u) \right] = f_0. \tag{15}$$

The second term, however, is inexact,

$$\begin{aligned} \int_\Omega \sum_{i=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) du &= R_k + \sum_{\ell=0}^{L} w_\ell \sum_{i=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u_\ell) && (16) \\ &= R_k + Q_k \left[\sum_{i=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) \right] && (17) \end{aligned}$$

where R_k is the residual, given by

$$R_k = \int_\Omega f(u) du - f_0 - Q_k \left[\sum_{i=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) \right]. \tag{18}$$

Thus, the error in the first moment using an index set Λ_k is given by

$$\begin{aligned} \mathbb{E}[f(u)] - \mathbb{E}[f(u)]_k &= f_0 + Q_k \left[\sum_{i=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) \right] + R_k - f_0, && (19) \\ &= Q_k \left[\sum_{i=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) \right] + R_k. && (20) \end{aligned}$$

As $\Lambda_k \to \Lambda_\infty$, the first term in the difference should vanish, as will R_k.

3 Ayres-Eaton

In similar fashion we consider the second moment convergence,

$$g_k = \frac{Q_k f^2 - Q_{k-1} f^2}{Q_{k-1} f^2}, \tag{21}$$

$$\mathbb{E}[f(u)^2] = \int_\Omega f(u)^2 du. \tag{22}$$

We again expand $f(u)$ in multidimensional orthogonal polynomials,

$$\begin{aligned} \mathbb{E}[f(u)^2] &= \int_\Omega \left[\sum_{i=0}^{\infty} f_{k_i} \Phi_{k_i}(u) \right]^2 du, && (23) \\ &= \int_\Omega \left[\sum_{i=0}^{J} f_{k_i} \Phi_{k_i}(u) + \sum_{i=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) \right]^2 du, && (24) \end{aligned}$$

$$= \int_\Omega \left[\sum_{i=0}^{J} \sum_{j=0}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) \right. \tag{25}$$

$$+ 2 \sum_{i=0}^{J} \sum_{j=J+1}^{\infty} f_{k_i} \Phi_{k_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) \tag{26}$$

$$\left. + \sum_{i=J+1}^{\infty} \sum_{j=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) \right] du. \tag{27}$$

Of the three sum-product terms above, only the first (Eq. **??**) will have any terms in which the overall polynomial order is small enough to integrate exactly using quadrature set Q_k. We split this term as

$$\int_\Omega \sum_{i=0}^{J} \sum_{j=0}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) du = \int_\Omega \left[\sum_{i=0}^{J} \sum_{j=0}^{J-i} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) + \sum_{i=0}^{J} \sum_{j=J-i+1}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) \right] du. \tag{28}$$

Using quadrature and because of orthogonality, the first term reduces to

$$\int_\Omega \sum_{i=0}^{J} \sum_{j=0}^{J-i} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) = Q_k \left[\sum_{i=0}^{J} \sum_{j=0}^{J-i} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) \right], \tag{29}$$

$$= \sum_{i=0}^{J/2} f_{k_i}^2. \tag{30}$$

The second term will have some residual error $R_{k,1}$ from inaccurate quadrature integration, as

$$\int_\Omega \sum_{i=0}^{J} \sum_{j=J-i+1}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) du = R_{k,1} + Q_k \left[\sum_{i=0}^{J} \sum_{j=J-i+1}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) \right]. \tag{31}$$

Thus, the term in Eq. **??** can be rewritten as

$$\int_\Omega \sum_{i=0}^{J} \sum_{j=0}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) du = \sum_{i=0}^{J/2} f_{k_i}^2 + R_{k,1} + Q_k \left[\sum_{i=0}^{J} \sum_{j=J-i+1}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) \right]. \tag{32}$$

None of the remaining terms (Eqs. **??**, **??**) can be integrated exactly using Q_k. By term, this results in

$$\int_\Omega 2 \sum_{i=0}^{J} \sum_{j=J+1}^{\infty} f_{k_i} \Phi_{k_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) du = 2R_{k,2} + 2Q_k \left[\sum_{i=0}^{J} \sum_{j=J+1}^{\infty} f_{k_i} \Phi_{k_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) \right], \tag{33}$$

$$\int_\Omega \sum_{i=J+1}^{\infty} \sum_{j=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) du = R_{k,3} + Q_k \left[\sum_{i=J+1}^{\infty} \sum_{j=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) \right]. \tag{34}$$

The second moment, then, is given by

$$\mathbb{E}[f(u)^2] = \sum_{i=0}^{J/2} f_{k_i}^2 \tag{35}$$

$$+ Q_k \left[\sum_{i=0}^{J} \sum_{j=J-i+1}^{J} f_{k_i} \Phi_{k_i}(u) f_{k_j} \Phi_{k_j}(u) \right] \tag{36}$$

$$+ 2Q_k \left[\sum_{i=0}^{J} \sum_{j=J+1}^{\infty} f_{k_i} \Phi_{k_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) \right] \tag{37}$$

$$+ Q_k \left[\sum_{i=J+1}^{\infty} \sum_{j=J+1}^{\infty} f_{\tilde{k}_i} \Phi_{\tilde{k}_i}(u) f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) \right] \tag{38}$$

$$+ R_{k,1} + 2R_{k,2} + R_{k,3}. \tag{39}$$

The three integration terms as well as the residuals should vanish as $\Lambda_k \to \Lambda_\infty$.

4 L2 of coefficient diffs

$$g_k = \sqrt{\sum_{i \in \Lambda_k} \left(f_{k_i}^{(k)} - f_{k_i}^{(k-1)} \right)^2}, \tag{40}$$

$$f_{k_i} = \int_\Omega f(u) \Phi_{k_i}(u) du, \tag{41}$$

$$= \int_\Omega \Phi_{k_i}(u) \sum_{j=0}^{\infty} f_{k_j} \Phi_{k_j}(u) du, \tag{42}$$

$$= \int_\Omega \Phi_{k_i}(u) \left[\sum_{j=0}^{J-k_i} f_{k_j} \Phi_{k_j}(u) + \sum_{j=J-k_j+1}^{\infty} f_{\tilde{k}_j} \Phi_{\tilde{k}_j}(u) \right] du. \tag{43}$$

The first term is integrated exactly by Q_k,

$$\int_\Omega \Phi_{k_i}(u) \sum_{j=0}^{J-i} f_{k_j} \Phi_{k_j}(u) du = Q_k \left[\Phi_{k_i}(u) \sum_{j=0}^{J-i} f_{k_j} \Phi_{k_j}(u) \right]. \tag{44}$$

If $2i \leq J$, this simplifies to f_i. Otherwise, this first term is zero. In either case, the second term is not integrated exactly,

$$\int_\Omega \Phi_{k_i}(u) \sum_{j=J-k_1}^{\infty} f_{k_j} \Phi_{k_j}(u) du = Q_k \left[\Phi_{k_i}(u) \sum_{j=J-k_1}^{\infty} f_{k_j} \Phi_{k_j}(u) \right] + R_{k_i}. \tag{45}$$