A brief note on sparse quadrature

Alen Alexanderian*

Abstract

We provide a brief introduction to sparse grids for computing integrals of multivariate functions.

1 Multivariate quadrature formulas

Consider $f : S \to \mathbb{R}$, with $S = [-1, 1]^d$, where d is an integer greater than one. We consider the problem of computing $\int_S f(\boldsymbol{x})\, d\boldsymbol{x}$. We use univariate quadrature formulas of the form

$$I^1_\ell(g) = \sum_{i=1}^{N_\ell} w^{(i,\ell)} g(x^{(i,\ell)}), \tag{1.1}$$

as the building blocks for constructing higher dimensional quadrature formulas. Here ℓ indicates the resolution level of the quadrature rule. The most straightforward approach is a full-tensor construction. For simplicity, let's consider the case where we use the I^1_ℓ in each coordinate direction. We can define,

$$I^d_{\mathrm{FT}}(f) = \sum_{i_1=1}^{N_\ell} \cdots \sum_{i_d=1}^{N_\ell} \left(\prod_{k=1}^{d} w^{(i_k,\ell)} \right) f(x_1^{(i_1,\ell)}, \ldots, x_d^{(i_d,\ell)}) =: (I^1_\ell \otimes \cdots \otimes I^1_\ell) f. \tag{1.2}$$

Notice that the number of nodes in this quadrature formula is $(N_\ell)^d$; this exponential scaling of the number of quadrature nodes with respect to d is often referred to as the *curse of dimensionality*.

As a concrete example of full-tensor grid, we can use the univariate n-point Gauss–Legendre rule, $I^1_n(g) = \sum_{j=1}^n w^{(j)} g(x^{(j)})$ to construct a full-tensor quadrature. In the case of $d = 2$, the full-tensor quadrature formula is as follows:

$$I^2_{\mathrm{FT},n}(f) = \sum_{i=1}^{n} \sum_{j=1}^{n} w^{(i)} w^{(j)} f(x_1^{(i)}, x_2^{(j)}).$$

Due to the curse of dimensionality, applicability of full-tensor quadrature formulas is limited to small dimensions (e.g., $d \le 8$ or so).

2 Sparse quadrature

Consider univariate rules of the form (1.1) for approximating $I(g) = \int_{-1}^{1} g(x)\, dx$. For $\ell \ge 1$, we define difference formulas

$$\Delta^1_\ell(g) = I^1_\ell(g) - I^1_{\ell-1}(g),$$

with $I^1_0 = 0$. Notice that (1.1) can be written as $I^1_\ell(g) = \sum_{i=1}^{\ell} \Delta^1_i(g)$. Also, assuming $E_\ell(g) = I^1_\ell(g) - I(g) \to 0$, as $\ell \to \infty$, we also have $\Delta^1_\ell(g) \to 0$, as $\ell \to \infty$. In particular, when using Gaussian quadrature formulas, the smoother g, the faster $\Delta^1_\ell(g)$ approaches zero, as ℓ increases.

Now, let us rewrite (1.2) using the difference formula just introduced:

$$\begin{aligned} I^d_{\mathrm{FT}}(f) = (I^1_\ell \otimes \cdots \otimes I^1_\ell) f &= \left(\big(\sum_{i_1=1}^{\ell} \Delta^1_{i_d} \big) \otimes \cdots \otimes \big(\sum_{i_d=1}^{\ell} \Delta^1_{i_d} \big) \right) f \\ &= \sum_{i_1=1}^{\ell} \cdots \sum_{i_d=1}^{\ell} (\Delta^1_{i_1} \otimes \cdots \Delta^1_{i_d}) f = \sum_{|\mathbf{i}|_\infty \le \ell} (\Delta^1_{i_1} \otimes \cdots \otimes \Delta^1_{i_d}) f. \end{aligned}$$

*North Carolina State University, Raleigh, NC, USA. E-mail: alexanderian@ncsu.edu
Last revised: March 3, 2018..

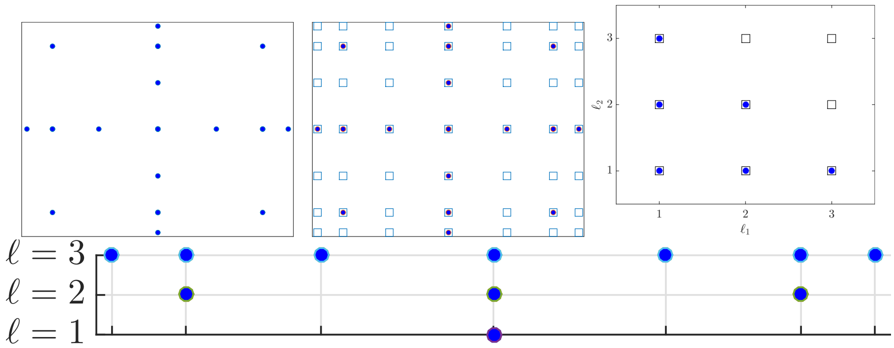

Figure 1: Top left: Level 3 sparse grid obtained using univariate Gauss-Kronrod-Patterson rule; top middle: the corresponding full-tensor grid (squares) with the sparse grid (filled dots) superimposed; top right: the sparse grid multi-index set $|(i_1, i_2)| \le 4$ (filled dots) and the full-tensor multi-index set $|(i_1, i_2)|_\infty \le 3$ (hollow squares). Bottom: Nodes of quadrature formulas I_1^1, I_2^1, and I_3^1.

Here $|\mathbf{i}|_\infty = \max_{1\le k\le d} i_k$. Sparse quadrature rules are obtained by retaining a subset of the terms of the above summation. Denoting $|\mathbf{i}|_1 = \sum_{k=1}^d i_k$, the classical Smolyak construction [1] is given by,

$$I^d_{\mathrm{smol},\ell}(f) = \sum_{|\mathbf{i}|_1 \le \ell+d-1} (\Delta^1_{i_1} \otimes \cdots \otimes \Delta^1_{i_d}) f.$$

For detailed description of computing the nodes and weights of a sparse quadrature formula, see [1]. As an illustration, we demonstrate the construction of a sparse quadrature formula for $d = 2$ and $\ell = 3$:

$$I^2_{\mathrm{smol},3} = \sum_{|\mathbf{i}|_1 \le 4} (\Delta^1_{i_1} \otimes \Delta^1_{i_2}) = (\Delta^1_1 \otimes \Delta^1_1) + (\Delta^1_1 \otimes \Delta^1_2) + (\Delta^1_2 \otimes \Delta^1_1) + (\Delta^1_2 \otimes \Delta^1_2) + (\Delta^1_1 \otimes \Delta^1_3) + (\Delta^1_3 \otimes \Delta^1_1).$$

We show in Figure 1 (top left) the nodes of level 3 sparse quadrature, obtained by using univariate Gauss-Kronrod-Patterson rule that is a nested variant of Gaussian quadrature [2]. The corresponding full-tensor grid is displayed in Figure 1 (top middle), with the sparse grid superimposed. The corresponding multi-index sets are depicted in Figure 1 (top right). The nodes of the univariate quadrature formulas corresponding to levels $\ell = 1, 2$, and 3 are shown in Figure 1 (bottom).

3 Further thoughts

In practice, the nodes and weights of full-tensor or sparse quadrature formulas are typically precomputed and ordered so as to write the quadrature formulas as

$$\int_S f(\boldsymbol{x})\, d\boldsymbol{x} \approx \sum_{j=1}^N W_j f(\boldsymbol{X}_j),$$

where $\boldsymbol{X}_j \in S$, and W_j, $j = 1, \ldots, N$ are the multi-dimensional quadrature nodes and weights.

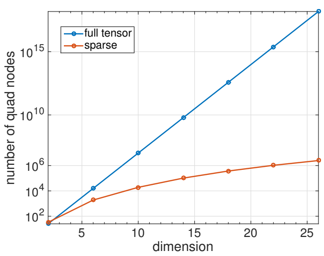

Figure 2: Nodes vs dimension.

The textbook [3] has a detailed, yet accessible discussion of sparse quadrature. It is also worth pointing out that sparse grid interpolation schemes can be developed analogously to the sparse grid quadrature rules; see e.g., [3]. Note that, while sparse grid formulas provide a significant improvement over the full-tensor quadrature (and interpolation) formulas as dimension increases (see e.g.,Figure 2), they *do not* solve the curse of dimensionality; sparse quadrature merely tempers the curse of dimensionality, and becomes impractical before d reaches around 40 or so, which is still not really a very high-dimensional problem in real applications. Adaptive sparse grids [4] can enable integration (interpolation) of higher-dimensional functions. However, for computing integrals of very high dimensional functions quasi Monte Carlo and Monte Carlo integration techniques can provide viable options, especially in the cases of non-smooth integrands.

References

[1] Gerstner, Thomas, and Michael Griebel. "Numerical integration using sparse grids." Numerical algorithms 18, 1998.

[2] Heiss, Florian, and Viktor Winschel. "Likelihood approximation by numerical integration on sparse grids." journal of Econometrics 144(1), 2008.

[3] Ralph C Smith. *Uncertainty quantification: theory, implementation, and applications*, volume 12. Siam, 2013.

[4] Gerstner, Thomas, and Michael Griebel. "Dimension-adaptive tensor-product quadrature." Computing, 71(1), 2003.