Quadrature using sparse grids on products of spheres

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Topics

- Weighted tensor product spaces on spheres
- Component-by-component construction
- Variations on sparse grid quadrature
- What's left to do?

Polynomials on the unit sphere

Sphere $\mathbb{S}^s := \{x \in \mathbb{R}^{s+1} \mid \sum_{k=1}^{s+1} x_k^2 = 1\}$.

$\mathbb{P}_\mu^{(s+1)}$: spherical polynomials of degree at most μ.

$\mathbb{H}_\ell^{(s+1)}$: spherical harmonics of degree ℓ, dimension $N_\ell^{(s+1)}$.

$\mathbb{P}_\mu^{(s+1)} = \bigoplus_{\ell=0}^{\mu} \mathbb{H}_\ell^{(s+1)}$ has spherical harmonic basis

$$\{Y_{\ell,k}^{(s+1)} \mid \ell \in 0 \ldots \mu, k \in 1 \ldots N_\ell^{(s+1)}\}.$$

Function space $H_{1,\gamma}^{(s,r)}$ on a single sphere

For $f \in L_2(\mathbb{S}^s)$, $f(x) \sim \sum_{\ell=0}^{\infty} \sum_{k=1}^{N_\ell^{(s+1)}} \hat{f}_{\ell,k} Y_{\ell,k}^{(s+1)}(x)$.

For positive weight γ, Reproducing Kernel Hilbert Space

$$H_{1,\gamma}^{(s,r)} := \{f : \mathbb{S}^s \to \mathbb{R} \mid \|f\|_{1,\gamma} < \infty\},$$

where $\|f\|_{1,\gamma} := \langle f, f \rangle_\gamma^{1/2}$ and

$$\langle f, g \rangle_{1,\gamma} := \sum_{\ell=0}^{\infty} \sum_{k=1}^{N_\ell^{(s+1)}} B_{s,r,\gamma}(\ell) \hat{f}_{\ell,k} \hat{g}_{\ell,k},$$

$$B_{s,r,\gamma}(\ell) := \quad 1 \text{ (if } \ell = 0\text{)}; \quad \gamma^{-1}\big(\ell(\ell+s-1)\big)^r \text{ (if } \ell \geq 1\text{)}.$$

(Kuo and Sloan, 2005)

Reproducing kernel of $H_{1,\gamma}^{(s,r)}$

This is

$$\begin{aligned} K_{1,\gamma}^{(s,r)}(x,y) &:= \sum_{\ell=0}^{\infty} \sum_{k=1}^{N_\ell^{(s+1)}} \frac{Y_{\ell,k}^{(s+1)}(x) Y_{\ell,k}^{(s+1)}(y)}{B_{s,r,\gamma}(\ell)} \\ &= 1 + \gamma A_{s,r}(x \cdot y), \quad \text{where for } z \in [-1,1], \\ A_{s,r}(z) &:= \sum_{\ell=1}^{\infty} \frac{N_\ell^{(s+1)}}{\big(\ell(\ell+s-1)\big)^r} \widetilde{C}_\ell^{(\frac{s-1}{2})}(z), \end{aligned}$$

with normalized ultraspherical polynomial

$$\widetilde{C}_\ell^{\lambda}(z) := \frac{C_\ell^{\lambda}(z)}{C_\ell^{\lambda}(1)}.$$

(Kuo and Sloan, 2005)

The weighted tensor product space $H^{(s,r)}_{d,\gamma}$

For $\gamma := (\gamma_1, \ldots, \gamma_d)$, on $(\mathbb{S}^s)^d$ define the tensor product space

$$H^{(s,r)}_{d,\gamma} := \bigotimes_{j=1}^{d} H^{(s,r)}_{1,\gamma_j}.$$

For $f \in H^{(s,r)}_{d,\gamma}, \quad x = (x_1, \ldots, x_d) \in (\mathbb{S}^s)^d$,

$f(x) = \sum_{\ell \in \mathbb{N}^d} \sum_{k \in \mathcal{K}(d,\ell)} \hat{f}_{\ell,k} \prod_{j=1}^{d} Y^{(s+1)}_{\ell_j,k_j}(x_j)$, where

$\mathcal{K}(d,\ell) := \{k \in \mathbb{N}^d \mid k_j \in 1 \ldots N^{(s+1)}_{\ell_j}$ for $j \in 1 \ldots d\}$.

Reproducing kernel of $H^{(s,r)}_{d,\gamma}$ is

$$K_{d,\gamma}(x,y) := \prod_{j=1}^{d} K^{(s,r)}_{1,\gamma_j}(x_j, y_j) = \prod_{j=1}^{d} \left(1 + \gamma_j A_{s,r}(x_j \cdot y_j)\right).$$

(Kuo and Sloan, 2005)

Equal weight quadrature error on $H^{(s,r)}_{d,\gamma}$

Worst case error of equal weight quadrature $Q_{m,d}$ with m points:

$$
\begin{aligned}
e^2_{m,d}(Q_{m,d}) &= -1 + \frac{1}{m^2} \sum_{i=1}^{m} \sum_{h=1}^{m} K_{d,\gamma}(x_i, x_h) \\
&= -1 + \frac{1}{m^2} \sum_{i=1}^{m} \sum_{h=1}^{m} \prod_{j=1}^{d} \big(1 + \gamma_j A_{s,r}(x_{i,j} \cdot x_{h,j})\big), \\
E(e^2_{m,d}) &= \frac{1}{m} \Big(-1 + \prod_{j=1}^{d} \big(1 + \gamma_j A_{s,r}(1)\big) \Big) \\
&\leq \frac{1}{m} \exp\big(A_{s,r}(1) \sum_{j=1}^{d} \gamma_j\big).
\end{aligned}
$$

(Kuo and Sloan, 2005)

Spherical designs on $\mathbb{S}^s$

A spherical design of strength t on $\mathbb{S}^s$ is an equal weight quadrature rule Q with m points $(x_1, \ldots, x_m)$, $Qf := \sum_{k=1}^{m} f(x_k)$, such that, for all $p \in \mathbb{P}_t(\mathbb{S}^s)$,

$$Q\,p = \int_{\mathbb{S}^s} p(y)\,d\omega(y)/|\mathbb{S}^s|.$$

The linear programming bounds give $t = \mathrm{O}(m^{1/d})$.

On the sphere $\mathbb{S}^2$ spherical designs of strength t are known to exist for $m = \mathrm{O}(t^3)$ and conjectured for $m = (t+1)^2$. Spherical t-designs have recently been found numerically for $m \geq (t+1)^2/2 + \mathrm{O}(1)$ for t up to 126.

(Delsarte, Goethals and Seidel, 1977; Hardin and Sloane, 1996; Chen and Womersley, 2006; Womersley, 2008)

Construction using permutations

The idea of Hesse, Kuo and Sloan, 2007 for quadrature on $(\mathbb{S}^2)^d$ is to use a spherical design $z = (z_1, \ldots, z_m)$ of strength t for the first sphere and then successively permute the points of the design to obtain the coordinates for each subsequent sphere.

The algorithm chooses permutations $\Pi_1, \ldots, \Pi_d : 1 \ldots m \to 1 \ldots m$, giving

$$x_i = (z_{\Pi_1(i)}, \ldots, z_{\Pi_d(i)})$$

to ensure that the resulting squared worst case quadrature error is better than the average $E(e^2_{m,d})$.

(Hesse, Kuo and Sloan, 2007)

Error estimate for permutation construction

Hesse, Kuo and Sloan prove that if $(z_1, \ldots, z_m)$ is a spherical t-design with $m = \mathrm{O}(t^2)$ or if $r > 3/2$ and $m = \mathrm{O}(t^3)$ for t large enough, then

$$D_m^2 := e^2_{m,1|_{\gamma_1 = 1}} = \frac{1}{m^2} \sum_{i=1}^{m} \sum_{h=1}^{m} A_{2,r}(z_{\Pi_j(i)} \cdot z_{\Pi_j(h)}) \leq \frac{A_{2,r}(1)}{m}.$$

This ensures that for m large enough, $M^2_{m,d}$, the average squared worst case error over all permutations, satisfies

$$M^2_{m,d} \leq E(e^2_{m,d}).$$

(Hesse, Kuo and Sloan, 2007)

Weighted Korobov spaces

Consider $s = 1$. $H^{(1,r)}_{1,\gamma}$ is a RKHS on the unit circle,

$H^{(1,r)}_{d,\gamma}$ is a RKHS on the d-torus.

This is a weighted Korobov space of periodic functions on $[0, 2\pi)^d$.

The Hesse, Kuo and Sloan construction in these spaces gives a rule with the same 1-dimensional projection properties as a lattice rule: the points are equally spaced.

(Wasilkowski and Woźniakowski, 1999; Hesse, Kuo and Sloan, 2007)

The Smolyak construction on $H_{d,1}^{(1,r)}$

The Smolyak construction and variants have been well studied on unweighted and weighted Korobov spaces.

Smolyak construction (unweighted case):
For $H_{1,1}^{(1,r)}$, define $Q_{1,-1} := 0$ and define a sequence of equal weight rules $Q_{1,0}, Q_{1,1}, \ldots$ on $[0, 2\pi)$, exact for trigonometric polynomials of degree $t_0 = 0 < t_1 < \ldots$.

Define $\Delta_q := Q_{1,q} - Q_{1,q-1}$ and for $H_{d,1}^{(1,r)}$, define

$$Q_{d,q} := \sum_{0 \leq a_1 + \ldots + a_d \leq q} \Delta_{a_1} \otimes \ldots \otimes \Delta_{a_d}.$$

(Smolyak, 1963; Wasilkowski and Woźniakowski, 1995; Gerstner and Griebel, 1998)

Smolyak vs lattice rules on $H_{d,1}^{(1,r)}$

Frank and Heinrich (1996) computes a discrepancy equivalent to the worst case error of quadrature on $H_{d,1}^{(1,r)}$.

Smolyak quadrature using the trapezoidal rule is compared to the rank 1 lattice rules of Haber (1983) and the rank 2 lattice rules of Sloan and Walsh (1990), in 3, 4 and 6 dimensions.

In all cases, the rank 2 rule outperforms the rank 1 rule, which beats the Smolyak-trapezoidal rule.

(Haber, 1983; Sloan and Walsh, 1990; Frank and Heinrich, 1996)

The WTP variant of Smolyak on $H_{d,\gamma}^{(1,r)}$

The WTP algorithm of Wasilkowski and Woźniakowski (1999) generalizes Smolyak by allowing other choices for the index sets a. (W and W (1999) treats spaces of non-periodic functions.)

For $H_{d,\gamma}^{(1,r)}$, define

$$W_{d,n} := \sum_{a \in P_{n,d}(\gamma)} \Delta_{a_1} \otimes \ldots \otimes \Delta_{a_d},$$

where $P_{1,d}(\gamma) \subset P_{2,d}(\gamma) \subset \mathbb{N}^d$, $|P_{n,d}(\gamma)| = n$.

W and W (1999) suggests to define $P_{n,d}(\gamma)$ by including the n rules $\Delta_{a_1} \otimes \ldots \otimes \Delta_{a_d}$ with largest norm.

(Wasilkowski and Woźniakowski, 1999)

WTP algorithm using spherical designs

For $H_{d,\gamma}^{(s,r)}$ with $s > 1$, we can define a WTP algorithm based on spherical designs on $\mathbb{S}^s$. Consider $s = 2$. Define a sequence of equal weight rules $Q_0, Q_1, \ldots$ using spherical designs of increasing strength $t_0 = 0 < t_1 < \ldots$ and cardinality $m_0 = 1 < m_1 < \ldots$.

The Smolyak and WTP constructions then proceed as per $s = 1$.

One difference between $s = 1$ and $s = 2$ is that spherical designs are not nested.

(Wasilkowski and Woźniakowski, 1999)

Error estimate for a single product rule

Based on the estimates of Hesse, Kuo and Sloan (2007),

$$e^2_{m,1}(Q_{m,1}) = \frac{\gamma_1}{m^2} \sum_{i=1}^{m} \sum_{h=1}^{m} A_{2,r}(x_i \cdot x_h),$$

we obtain for the product rule $R := Q_{m_1,1} \otimes \ldots \otimes Q_{m_d,1}$,

$$\begin{aligned} e^2(R) &= -1 + \prod_{j=1}^{d} \frac{1}{m_j^2} \sum_{i=1}^{m_j} \sum_{h=1}^{m_j} \left(1 + \gamma_j A_{2,r}(x_{j_i} \cdot x_{j_h})\right) \\ &\leq -1 + \prod_{j=1}^{d} \left(1 + \frac{\gamma_j}{m_j} A_{2,r}(1)\right). \end{aligned}$$

(Hesse, Kuo and Sloan, 2007)

Error estimate for a single product rule

If $m := \prod_{j=1}^{d} m_j$ then we have

$$e^2(R) \leq \frac{1}{m}\left(-m + \prod_{j=1}^{d}\left(m_j + \gamma_j A_{2,r}(1)\right)\right)$$
$$\geq \frac{1}{m}\left(-1 + \prod_{j=1}^{d}\left(1 + \gamma_j A_{2,r}(1)\right)\right).$$

So this upper bound for such a product rule is worse than the average worst case error.

(Hesse, Kuo and Sloan, 2007)

Optimal linear combination of product rules

Since the Smolyak and WTP algorithms are based on tensor products of differences Δ_{a_j}, they are each equivalent to a specific linear combination of product rules $R_1, \ldots, R_N$.
We can instead find the coefficients α_k giving the best worst case error of $Q = \sum_{p=1}^{N} \alpha_p R_p$ by minimizing

$$\begin{aligned} e^2(Q) &= \langle I^* - Q^*, I^* - Q^* \rangle_{d,\gamma} \\ &= 1 - 2 \sum_{k=1}^{N} \alpha_p + \sum_{p=1}^{N} \sum_{q=1}^{N} \alpha_p \alpha_q \langle R_p^*, R_q^* \rangle_{d,\gamma}, \end{aligned}$$

where I^* is the representer of the integral on $(\mathbb{S}^2)^d$,
Q^* is the representer of the rule Q, etc.

(Kuo and Sloan, 2005)

Optimal linear combination of product rules

The squared error is quadratic in the α_p and stationary when

$$\sum_{q=1}^{N} \alpha_q \langle R_p^*, R_q^* \rangle_d = 1$$

for $p \in 1 \ldots N$.

(Larkin, 1970; Kuo and Sloan, 2005)

Almost everything is still to do

- Error estimates for tensor product algorithms.
  What is the improvement in error for the best linear combination of product rules over the best single product rule?
- Best rate of increase of strength of spherical designs.
  Should it double very step?
- Best index sets.
  What is the best way to take weights into account?
- Maximum determinant interpolatory quadrature rules.
  Are these better than spherical designs?
- Constraints on γ for strong tractability.
- Numerical experiments.
- Extension to higher dimensional spheres; other compact sets.