Quadrature using sparse grids on products of spheres

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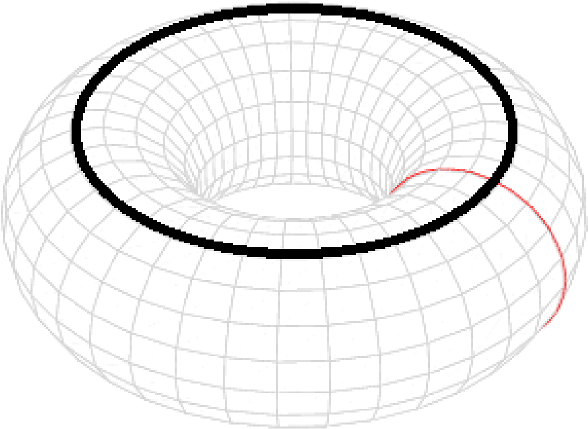
Topics

- Weighted tensor product spaces on spheres
- Component-by-component construction
- Weighted tensor product quadrature
- Numerical results
- Accomplishments and next steps

A product of two circles is a torus. . .



(‘Torus cycles” - Wikipedia, 2005)

Polynomials on the unit sphere

Sphere $\mathbb{S}^2 := \{x \in \mathbb{R}^3 \mid \sum_{k=1}^{3} x_k^2 = 1\}$.

$\mathbb{P}_\mu$: spherical polynomials of degree at most μ.

$\mathbb{H}_\ell$: spherical harmonics of degree ℓ, dimension $2\ell + 1$.

$\mathbb{P}_\mu = \bigoplus_{\ell=0}^{\mu} \mathbb{H}_\ell$ has spherical harmonic basis

$$\{Y_{\ell,k} \mid \ell \in 0 \ldots \mu, k \in 1 \ldots 2\ell + 1\}.$$

Reproducing kernel Hilbert space $\boldsymbol{H}$ on $\boldsymbol{X}$

A reproducing kernel Hibert space $\boldsymbol{H}$ of real functions on a manifold $\boldsymbol{X}$ is a Hilbert space with inner product $\langle , \rangle$ and a kernel

$$\boldsymbol{K} : \boldsymbol{X} \times \boldsymbol{X} \to \mathbb{R},$$

such that for all $\boldsymbol{x} \in \boldsymbol{X}$, if $\boldsymbol{k_x}$ is defined by

$$\boldsymbol{k_x}(\boldsymbol{y}) := \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{y}) \quad \text{for all } \boldsymbol{y} \in \boldsymbol{X}, \text{ then}$$
$$\boldsymbol{k_x} \in \boldsymbol{H} \quad \text{and} \quad \langle \boldsymbol{k_x}, \boldsymbol{f} \rangle = \boldsymbol{f}(\boldsymbol{x}) \text{ for all } \boldsymbol{f} \in \boldsymbol{H}.$$

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

For $f \in L_2(\mathbb{S}^2)$, $f(x) \sim \sum_{\ell=0}^{\infty} \sum_{k=1}^{2\ell+1} \hat{f}_{\ell,k} Y_{\ell,k}(x)$.

For positive weight γ, Reproducing Kernel Hilbert Space

$$H_{1,\gamma}^{(r)} := \{f : \mathbb{S}^2 \to \mathbb{R} \mid \|f\|_{1,\gamma} < \infty\},$$

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

$$\langle f, g \rangle_{1,\gamma} := \hat{f}_{0,0}\, \hat{g}_{0,0} + \gamma^{-1} \sum_{\ell=1}^{\infty} \sum_{k=1}^{2\ell+1} \big(\ell(\ell+1)\big)^{r} \hat{f}_{\ell,k}\, \hat{g}_{\ell,k}.$$

(Kuo and Sloan, 2005)

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

This is

$$K_{1,\gamma}^{(r)}(x,y) := 1 + \gamma A_r(x \cdot y), \quad \text{where for } z \in [-1,1],$$

$$A_r(z) := \sum_{\ell=1}^{\infty} \frac{2\ell+1}{\big(\ell(\ell+1)\big)^r} P_\ell(z),$$

where P is a Legendre polynomial.

(Kuo and Sloan, 2005)

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

For $\gamma := (\gamma_1, \ldots, \gamma_d)$, on $(\mathbb{S}^2)^d$ define the tensor product space

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

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

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

(Kuo and Sloan, 2005)

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

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

$$e^2_{m,d}(Q_{m,d}) := \sup_{f \in H^{(r)}_{d,\gamma}} ((\mathbb{I} - Q_{m,d})f)^2$$

$$= -1 + \frac{1}{m^2} \sum_{i=1}^{m} \sum_{h=1}^{m} K_{d,\gamma}(x_i, x_h)$$

$$= -1 + \frac{1}{m^2} \sum_{i=1}^{m} \sum_{h=1}^{m} \prod_{j=1}^{d} \left(1 + \gamma_j A_r(x_{i,j} \cdot x_{h,j})\right),$$

$$E(e^2_{m,d}) = \frac{1}{m}\left(-1 + \prod_{j=1}^{d} \left(1 + \gamma_j A_r(1)\right)\right)$$

$$\leq \frac{1}{m} \exp\left(A_r(1) \sum_{j=1}^{d} \gamma_j\right).$$

(Kuo and Sloan, 2005)

Spherical designs on $\mathbb{S}^2$

A spherical design of strength t on $\mathbb{S}^2$ 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 $p \in \mathbb{P}_t(\mathbb{S}^2)$,

$$Q\, p = \int_{\mathbb{S}^2} p(y)\, d\omega(y)/|\mathbb{S}^2|.$$

The linear programming bounds give $t = \mathrm{O}(m^{1/2})$.

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

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

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 $s = 1$. $H_{1,\gamma}^{(1,r)}$ is a RKHS on the unit circle $\mathbb{S}^1$,

$H_{d,\gamma}^{(1,r)}$ 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 $\mathbb{S}^1$

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)

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

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

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

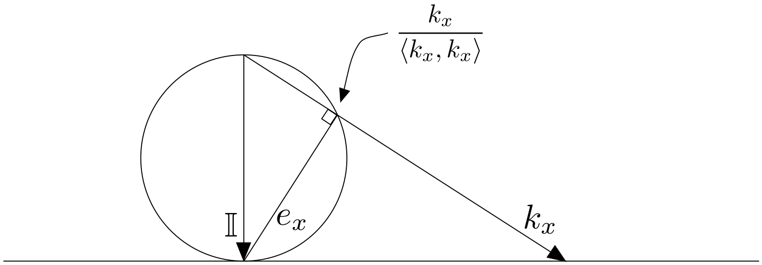
$$W_{d,n} := \sum_{a \in P_{n,d}(\gamma)} \Delta_{a_1} \otimes \ldots \otimes \Delta_{a_d},$$

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.

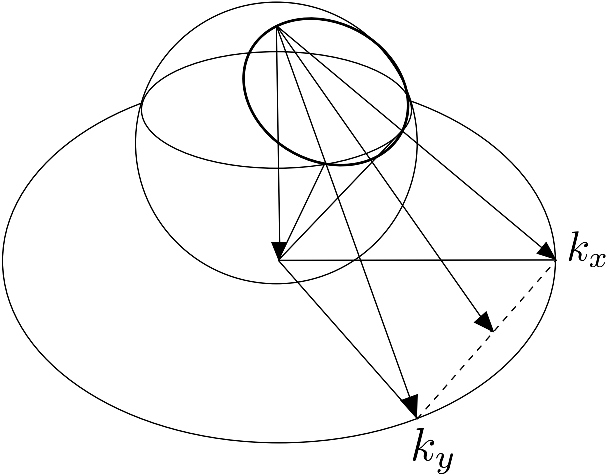
(Wasilkowski and Woźniakowski, 1999)

Optimal weight for one quadrature point



(Illustration by Osborn, 2009)

Optimal weights for two quadrature points



(Illustration by Osborn, 2009)

WTP rules using spherical designs

For $H_{d,\gamma}^{(r)}$ we can define a WTP rule based on spherical designs. Define a sequence of optimal weight rules $Q_0, Q_1, \ldots$ using unions of spherical designs of increasing strength $t_0 = 0 < t_1 < \ldots$ and cardinality $m_0 = 1 < m_1 < \ldots$.

The WTP construction then proceeds similarly to $\mathbb{S}^1$.

One difference between $\mathbb{S}^1$ and $\mathbb{S}^2$ is that the spherical designs themselves cannot be nested in general.

(Wasilkowski and Woźniakowski, 1999)

Generic WTP algorithm for $\mathbb{S}^2$

1. Begin with a sequence of spherical designs $X_1, X_2, \ldots X_L$, with increasing cardinality, nondecreasing strength.
2. For each h, form the optimal weight rule Q_h from the point set $\bigcup_{i=1}^{h} X_i$, and the difference rule $\Delta_h = Q_h - Q_{h-1}$.
3. Form products of the difference rules and rank them in decreasing norm (possibly weighted by the number of additional points).
4. Form WTP rules by adding product difference rules in rank order.

The Hesse, Kuo and Sloan example space

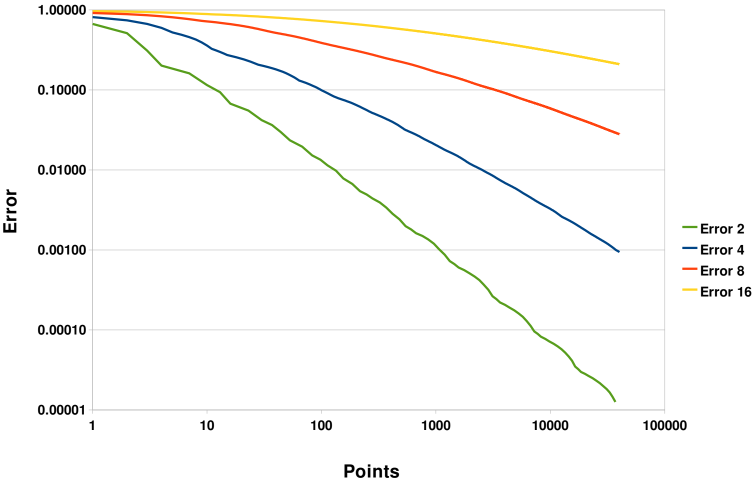
In Hesse, Kuo and Sloan, a numerical example is given with $r = 3$, $\gamma_j = 0.9^j$. In other words,

$$K_{d,\gamma}(x, y) := \prod_{j=1}^{d} K^{(3)}_{1,0.9^j}(x_j, y_j) = \prod_{j=1}^{d} \left(1 + 0.9^j A_3(x_j \cdot y_j)\right),$$

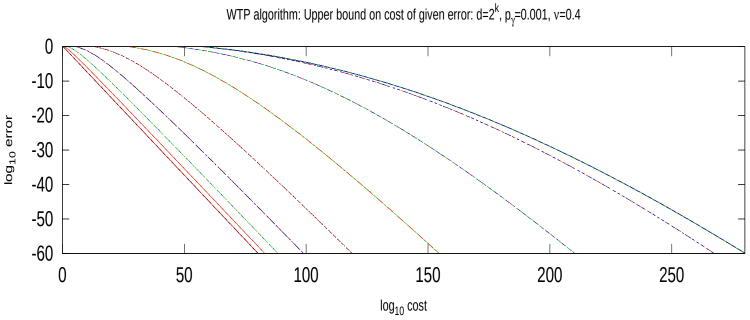
where

$$A_3(z) = \sum_{\ell=1}^{\infty} \frac{2\ell + 1}{\left(\ell(\ell+1)\right)^3} P_\ell(z).$$

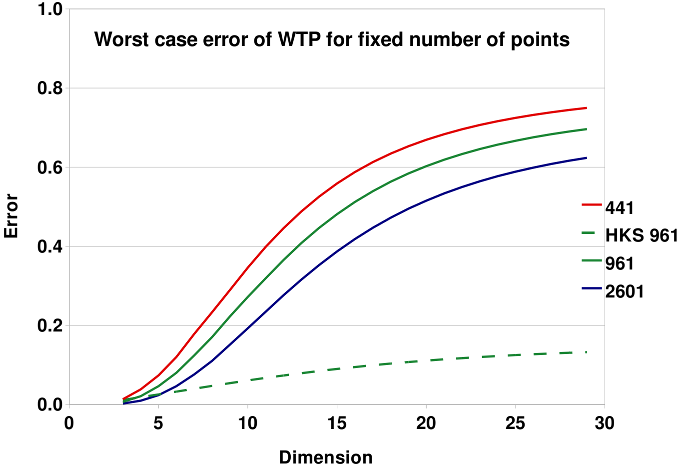
Error of WTP rule for $\mathbb{S}^2$



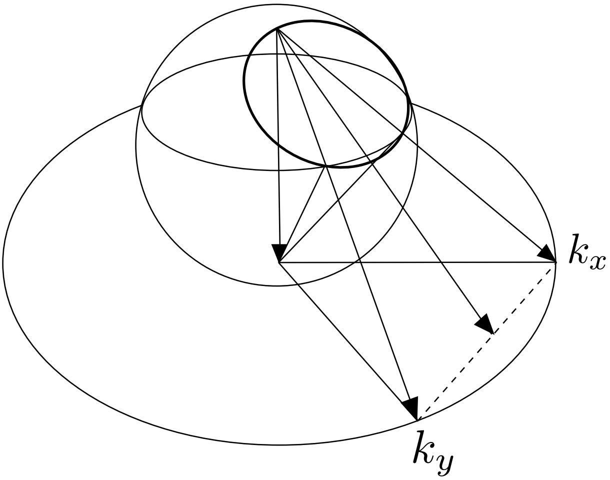
Estimated upper bound of error of WTP rule



Comparisons for 441, 961 and 2601 points



Weights for two quadrature points reconsidered



(Illustration by Osborn, 2009)

Accomplishments

- Formulation of WTP algorithm for products of $\mathbb{S}^2$.
- Implementation of WTP algorithm.
- Numerical results for d to 30 and up to $40\,000$ points.
- Estimate for upper bound of error of WTP rule.

To do

- More error estimates for WTP rules.
  Lower bounds on error; initial rate of convergence.
- Improvement of WTP algorithm to obtain better initial rate of convergence.
- 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?
- More numerical experiments.