The rate of convergence of sparse grid quadrature on products of spheres

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For presentation at MCQMC 2010 Warsaw Poland.
Joint work with Markus Hegland, ANU.

August 2010

AUSTRALIAN RESEARCH COUNCIL
Centre of Excellence for Mathematics
and Statistics of Complex Systems

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Topics

- Weighted tensor product spaces on spheres
- Component-by-component construction
- Weighted tensor product quadrature
- Numerical results
- Discussion

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 H on M

A Reproducing Kernel Hilbert Space (RKHS) H of real functions on a manifold M is a Hilbert space with inner product $\langle , \rangle$ and a kernel

$$K : M \times M \to \mathbb{R},$$

such that for all $x \in M$, if k_x is defined by

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

KS function space $H^{(r)}_{1,\gamma}$ 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, define the RKHS

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

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

This is

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

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

where P is a Legendre polynomial.

(Kuo and Sloan, 2005)

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

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

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

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

$$K_{d,\gamma}(x, y) := \prod_{j=1}^{d} K_{1,\gamma_j}^{(r)}(x_j, y_j)$$

(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:

$$e^2_{m,d}(Q_{m,d}) := \sup_{f \in H^{(r)}_{d,\gamma}} \left((\mathbb{I} - Q_{m,d})f\right)^2$$
$$= -1 + \frac{1}{m^2} \sum_{i=1}^{m} \sum_{h=1}^{m} K_{d,\gamma}(x_i, x_h).$$

Expected squared error satisfies:

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

(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 proved 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

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

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 on $(\mathbb{S}^1)^d$

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

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

General quadrature weights on $H^{(2,r)}_{d,\gamma}$

For $X := \{x_1, \ldots, x_m\}$, if we define

$$Q_w f := \sum_{k=1}^{m} w_k f(x_k),$$
$$G_{i,j} := \langle k_{x_i}, k_{x_j} \rangle = K_{d,\gamma}(x_i, x_j),$$

then the worst case error e_w for Q_w satisfies

$$e_w^2 = \|1 - Q_w\|^2 = \langle 1 - Q_w, 1 - Q_w \rangle$$
$$= 1 - 2\sum_{k=1}^{m} w_k + w^T G w.$$

Optimal quadrature weights on $H^{(2,r)}_{d,\gamma}$

Since

$$e_w^2 = 1 - 2\sum_{k=1}^{m} w_k + w^T G w,$$

the weights w are optimal when $Gw = [1, \ldots, 1]^T$.

In this case, $e_w^2 = 1 - \sum_{k=1}^{m} w_k$.

The Smolyak construction on $(\mathbb{S}^1)^d$

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

Smolyak construction (unweighted Korobov space case):
For $H^{(1,r)}_{1,1}$, 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 $H^{(1,r)}_{d,1}$, 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)

WTP rules using spherical designs

For $H^{(r)}_{d,\gamma}$ 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 $\boldsymbol{X_1, X_2, \ldots X_L}$, with increasing cardinality, nondecreasing strength.
2. For each $\boldsymbol{h}$, form the optimal weight rule $\boldsymbol{Q_h}$ from the point set $\bigcup_{i=1}^{h} \boldsymbol{X_i}$, and the difference rule $\boldsymbol{\Delta_h = Q_h - Q_{h-1}}$.
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

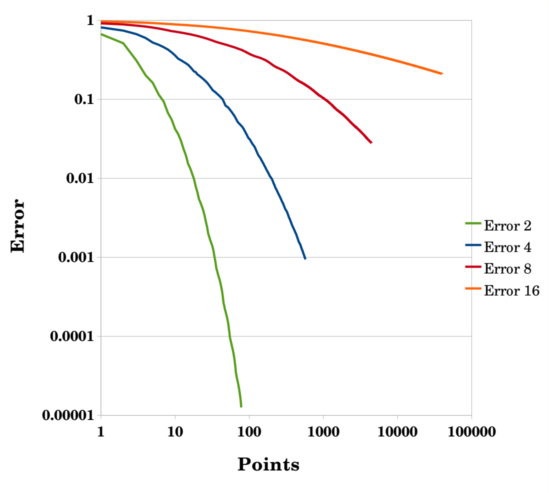
In Hesse, Kuo and Sloan, a numerical example is given with $r = 3$, $\gamma_j = 0.9^j$. In other words,

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

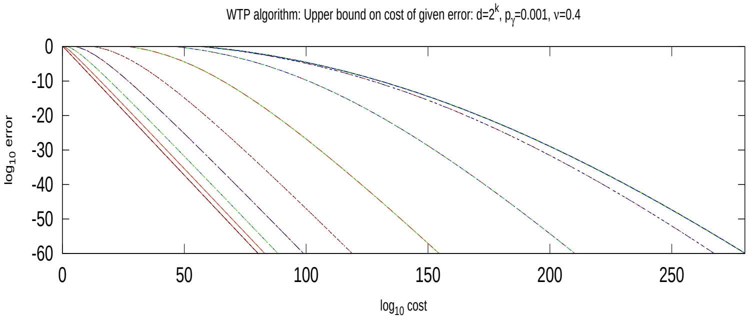
where

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

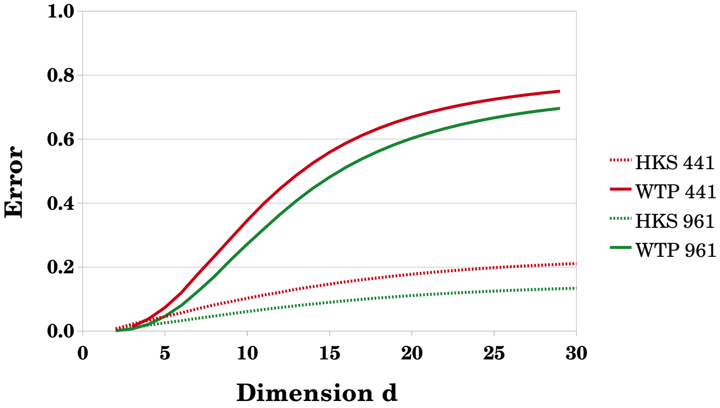
Error of WTP rule for $(\mathbb{S}^2)^d, d = 2, 4, 8, 16$



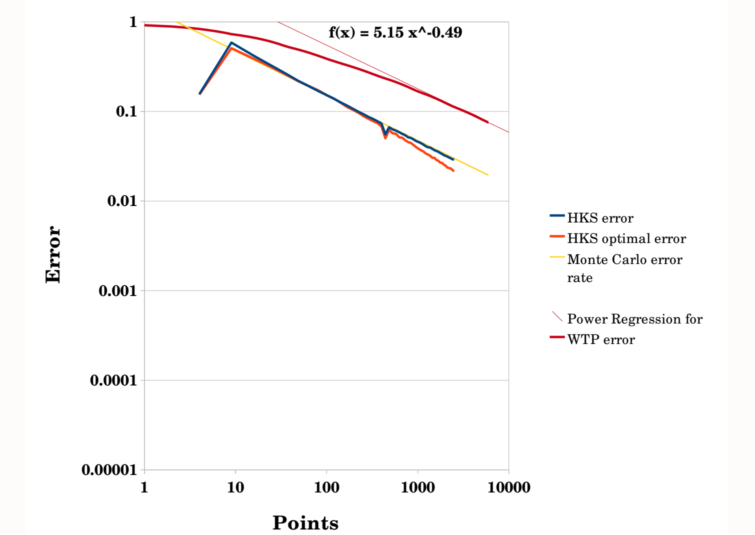
Estimated upper bound of error of WTP rule



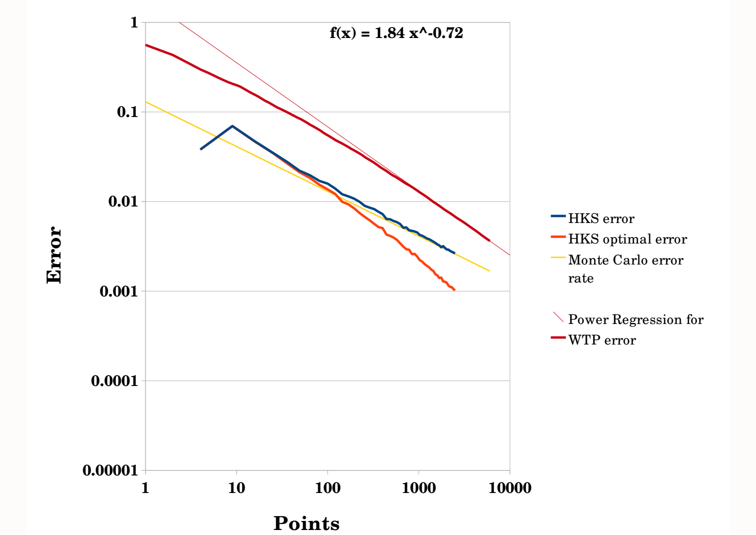
HKS vs WTP: 441, 961 points



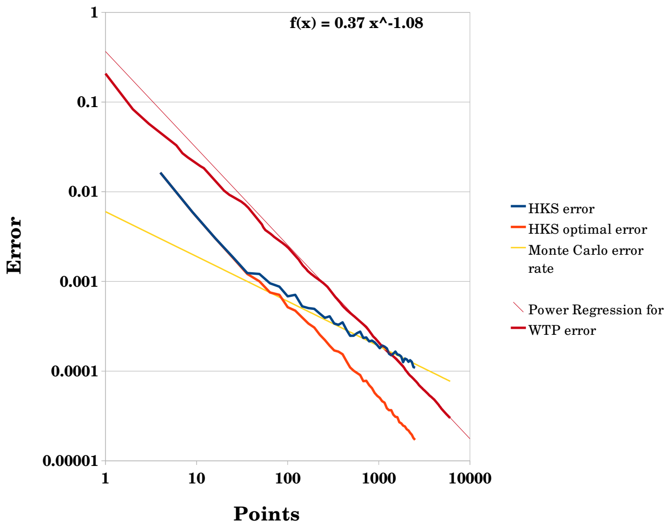
HKS vs WTP: $(\mathbb{S}^2)^8, r = 3, g = 0.9, \gamma = g^j$



HKS vs WTP: $(\mathbb{S}^2)^8, r = 3, g = 0.5, \gamma = g^j$



HKS vs WTP: $(\mathbb{S}^2)^8, r = 3, g = 0.1, \gamma = g^j$



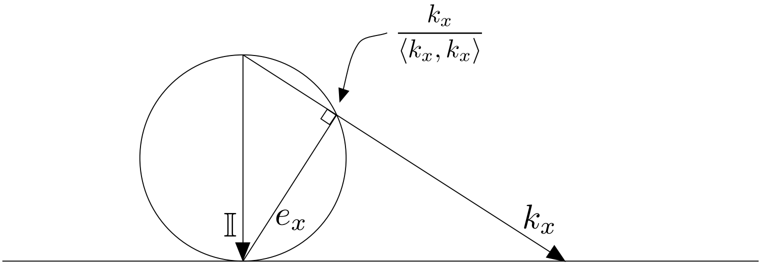
Why does WTP (initially) perform poorly?

WTP points are too close together.

- Partly because, for one sphere, nesting is forced.
- Mostly because, for higher d, initially only one sphere at a time is changed.

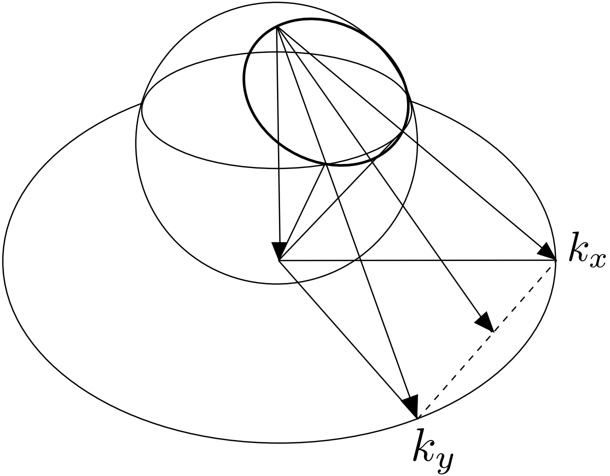
HKS points are better separated.

Optimal weight for one quadrature point



(Illustration by Osborn, 2009)

Optimal weights for two quadrature points



(Illustration by Osborn, 2009)