Sparse grid methods (continued)

Vesa Kaarnioja (kaarnioja@uni-mannheim.de)
Claudia Schillings (c.schillings@uni-mannheim.de)

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University of Mannheim

Short recap of last week

For any multi-index $\alpha \in \mathbb{N}^d$ (here $0 \in \mathbb{N}$), we define $|\alpha|_1 = \sum_{i=1}^d \alpha_i$ and $|\alpha|_\infty = \max_{1 \le i \le d} \alpha_i$.

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We consider the function spaces

$$H^r(\Omega) = \left\{ f : \Omega \to \mathbb{R};\ \frac{\partial^\alpha f(x)}{\partial x^\alpha} \text{ exists and is bounded in } \Omega \text{ for all } |\alpha|_\infty \le r \right\}$$

for a fixed region $\varnothing \neq \Omega \subseteq \mathbb{R}^d$. We call r the *regularity* of functions in $H^r(\Omega)$ and accompany these function spaces with the respective norms

$$||f||_{H^r(\Omega)} = \max_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha|_\infty \le r}} \sup \left\{ \left| \frac{\partial^\alpha f(x)}{\partial x^\alpha} \right|;\ x \in \Omega \right\}.$$

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Let $T : H^r(\Omega) \to \mathbb{R}$ be a bounded, linear functional. The *operator norm* of T is defined by

$$\|T\| := \sup_{\|f\|_{H^r(\Omega)} \le 1} |Tf|.$$

Naturally, $|Tf| \le \|T\| \|f\|_{H^r(\Omega)}$ for all $f \in H^r(\Omega)$.

Suppose that $\varnothing \neq \Omega \subseteq \mathbb{R}^{d_1}$ and $\varnothing \neq \Xi \subseteq \mathbb{R}^{d_2}$ and let $S\colon H^r(\Omega) \to \mathbb{R}$ and $T\colon H^r(\Xi) \to \mathbb{R}$ be functionals. Suppose additionally that they admit to representations

$$Sf = \sum_{i=1}^{m} a_i f(x_i) \quad \text{and} \quad T\tilde{f} = \sum_{i=1}^{n} b_i \tilde{f}(y_i)$$

for a selection of positive weights $(a_i)_{i=1}^m$ and $(b_i)_{i=1}^n$ and vectors $(x_i)_{i=1}^m$ and $(y_i)_{i=1}^n$ in the domains Ω and Ξ. Now $\Omega \times \Xi \subseteq \mathbb{R}^{d_1+d_2}$ and the *tensor product* of S and T is the linear functional $S \otimes T\colon H^r(\Omega \times \Xi) \to \mathbb{R}$ defined by setting

$$(S \otimes T)f = \sum_{i=1}^{m} \sum_{j=1}^{n} a_i b_j f(x_i, y_j).$$

During this lecture, we shall consider the sequence of univariate Clenshaw–Curtis quadrature rules $(U_i)_{i=1}^{\infty}$, which are of the form

$$U_i f = \sum_{j=1}^{m_i} w_j^i f(x_j^i), \quad f \in H^r([-1,1]^d).$$

The i^{th} CC rule has m_i-points, where $m_1 = 1$ and $m_i = 2^{i-1}+1$, $i > 1$. The nodes $(x_j^i)_{j=1}^{m_i}$ and weights $(w_j^i)_{j=1}^{m_i}$ of an m_i-point CC rule have explicit formulae

$$x_j^i = -\cos\left(\frac{\pi(j-1)}{m_i - 1}\right), \quad j \in \{1,\ldots,m_i\}$$

$$w_j^i = w_{m_i+1-j}^i = \begin{cases} \frac{1}{m_i(m_i-2)}, & j \in \{1, m_i\} \\ \frac{2}{m_i-1}\left(1 - \frac{\cos(\pi(j-1))}{m_i(m_i-2)} - 2\sum_{k=1}^{(m_i-3)/2} \frac{1}{4k^2-1}\cos\left(\frac{2\pi k(j-1)}{m_i-1}\right)\right) & \text{otherwise.} \end{cases}$$

The evaluation points of the CC rules are nested: Let us denote $X_i := \{x_j^i\}_{j=1}^{m_i}$. Then $X_i \subset X_{i+1}$ for all $i \geq 1$.

Properties of tensor products of linear functionals

- Noncommutative: generally $S \otimes T \neq T \otimes S$.
- Associative: $(S \otimes T) \otimes R = S \otimes (T \otimes R)$.
- Distributive: $(S + T) \otimes R = S \otimes R + T \otimes R$.

Theorem

Let T_i be quadrature operators. Then

$$\left\| \bigotimes_{i=1}^{n} T_i \right\| = \prod_{i=1}^{n} \| T_i \|$$

in their respective operator norms.

If $f(x, y) = g(x)h(y)$, then $(S \otimes T)f = Sg \cdot Th$.

Definition (Smolyak quadrature rule)

Let $(U_i)_{i=1}^{\infty}$ be a sequence of univariate quadrature rules in the interval $\varnothing \neq I \subseteq \mathbb{R}$. We introduce the *difference operators* by setting

$$\Delta_0 = 0, \quad \Delta_1 = U_1 \quad \text{and} \quad \Delta_{i+1} = U_{i+1} - U_i \quad \text{for } i = 1, 2, 3, \ldots .$$

The *Smolyak quadrature rule* of order k in the hyperrectangle $I^d = I \times \cdots \times I$ is the operator

$$\mathcal{Q}_k^d = \sum_{\substack{|\alpha|_1 \leq k \\ \alpha \in \mathbb{N}^d}} \bigotimes_{i=1}^{d} \Delta_{\alpha_i}. \tag{1}$$

The tensor product $\Delta_{\alpha_1} \otimes \cdots \otimes \Delta_{\alpha_d}$ in the summand of (1) vanishes whenever $\alpha_i = 0$ for some index i. In the sequel we always assume that $\alpha \geq \mathbf{1}$ and hence $k \geq d$.

Proposition (Dimension recursion)

Let $k \geq d \geq 2$. Then

$$\mathcal{Q}_k^d = \sum_{\substack{|\alpha|_1 \leq k-1 \\ \alpha \in \mathbb{N}^{d-1},\ \alpha \geq \mathbf{1}}} \left(\bigotimes_{i=1}^{d-1} \Delta_{\alpha_i} \right) \otimes U_{k-|\alpha|_1} = \sum_{i=d-1}^{k-1} \mathcal{Q}_i^{d-1} \otimes \Delta_{k-i}.$$

A (computationally) useful characterization:

Theorem (Combination method)

Let U_i be univariate quadrature rules in the interval $\varnothing \neq I \subseteq \mathbb{R}$ and suppose that $k \geq d$. Then

$$\mathcal{Q}_k^d = \sum_{\substack{\max\{d, k-d+1\} \leq |\alpha|_1 \leq k \\ \alpha \in \mathbb{N}^d,\ \alpha \geq \mathbf{1}}} (-1)^{k-|\alpha|_1} \binom{d-1}{k-|\alpha|_1} \bigotimes_{i=1}^{d} U_{\alpha_i}. \tag{2}$$

Exercise. Using the formula

$$\mathcal{Q}_k^d = \sum_{\substack{\max\{d,k-d+1\}\leq|\alpha|_1\leq k\\ \alpha\in\mathbb{N}^d,\ \alpha\geq\mathbf{1}}} (-1)^{k-|\alpha|_1}\binom{d-1}{k-|\alpha|_1}\bigotimes_{i=1}^{d} U_{\alpha_i}$$

expand the above expression to find the Smolyak quadrature rule $\mathcal{Q}_3^2$.

Next, plug the Clenshaw–Curtis quadrature rules

$$U_1 f = f(\tfrac{1}{2}) \quad \text{and} \quad U_2 f = \tfrac{1}{6}f(0) + \tfrac{2}{3}f(\tfrac{1}{2}) + \tfrac{1}{6}f(1)$$

into the formula you obtained for $\mathcal{Q}_3^2$ and derive a quadrature rule in the form

$$\mathcal{Q}_3^2 f = w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3) + w_4 f(x_4) + w_5 f(x_5),$$

where $(w_i)_{i=1}^5$ are weights and $(x_i)_{i=1}^5$ are elements in $[0,1]^2$.

Solution. You should obtain (akin to last week's example)

$$\mathcal{Q}_3^2 = U_1 \otimes U_2 + U_2 \otimes U_1 - U_1 \otimes U_1.$$

Substituting the Clenshaw–Curtis rules yields

$$\mathcal{Q}_3^2 f = \tfrac{1}{6} f(\tfrac{1}{2}, 0) + \tfrac{1}{6} f(\tfrac{1}{2}, 1) + \tfrac{1}{6} f(0, \tfrac{1}{2}) + \tfrac{1}{6} f(1, \tfrac{1}{2}) + \tfrac{1}{3} f(\tfrac{1}{2}, \tfrac{1}{2}).$$

Today, we consider the problem of approximating

$$\mathcal{I}^d f := \int_{[-1,1]^d} f(y_1,\dots,y_d)\,\mathrm{d}y_1\cdots\mathrm{d}y_d, \quad f\in H^r([-1,1]^d).$$

To this end, let us extend the definition of the tensor product as follows: if $Tf = \sum_{i=1}^n w_i f(x_i)$ for $f \in H^r([-1,1]^s)$, then we define

$$(T\otimes\mathcal{I}^d)f = \sum_{i=1}^n w_i \int_{[-1,1]^s} f(x_i,y)\,\mathrm{d}y$$

$$(\mathcal{I}^d\otimes T)f = \sum_{i=1}^n w_i \int_{[-1,1]^s} f(y,x_i)\,\mathrm{d}y$$

$$(\mathcal{I}^d\otimes\mathcal{I}^s)f = \int_{[-1,1]^{s+d}} f(x,y)\,\mathrm{d}x\,\mathrm{d}y$$

for $f\in H^r([-1,1]^{d+s})$. Note that $\|\mathcal{I}^d\otimes T\| = \|T\otimes\mathcal{I}^d\| = \|\mathcal{I}^d\|\|T\|$.

Some essential combinatorics

Lemma

$$\sum_{\substack{|\alpha|_1=k\\ \alpha\in\mathbb{N}^d,\ \alpha\geq\mathbf{1}}} 1 = \binom{k-1}{d-1} \quad \textit{and} \quad \sum_{\substack{|\alpha|_1\leq k\\ \alpha\in\mathbb{N}^d,\ \alpha\geq\mathbf{1}}} 1 = \binom{k}{d}.$$

Proof. The first identity follows from a combinatorial ("stars and bars") argument. The second identity follows from

$$\sum_{\substack{|\alpha|_1\leq k\\ \alpha\in\mathbb{N}^d,\ \alpha\geq\mathbf{1}}} 1 = \sum_{\ell=d}^{k} \sum_{\substack{|\alpha|_1=\ell\\ \alpha\in\mathbb{N}^d,\ \alpha\geq\mathbf{1}}} 1 = \sum_{\ell=d}^{k} \binom{\ell-1}{d-1} = \binom{k}{d},$$

where the final equality follows from the summation formula for the diagonals of Pascal's triangle (proof by induction and using Pascal's identity; omitted.) □

On the distribution of Smolyak quadrature nodes

The evaluation points of $\mathcal{Q}_k^d$ form the set

$$\eta(k,d) = \bigcup_{\substack{\max\{d,k-d+1\} \le |\alpha|_1 \le k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} X_{\alpha_1} \times \cdots \times X_{\alpha_d} \quad \text{for all } k \ge d.$$

The elements of the set $\eta(k,d)$ are the *nodes* of $\mathcal{Q}_k^d$.

If the univariate rules are nested, i.e., $X_i \subseteq X_{i+1}$ (as is the case with CC rules), then the nodes of $\mathcal{Q}_k^d$ form the set

$$\eta(k,d) = \bigcup_{\substack{|\alpha|_1 = k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} X_{\alpha_1} \times \cdots \times X_{\alpha_d} \quad \text{for all } k \ge d. \tag{3}$$

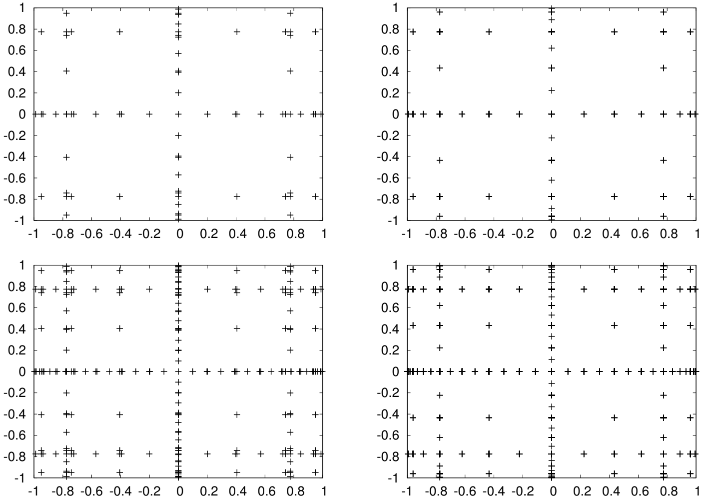

Figure: Left: non-nested Smolyak–Gauss–Legendre rules $\mathcal{Q}_k^d$ for $d = 2$ and $k \in \{5, 6\}$. Right: nested Smolyak–Gauss–Patterson rules $\mathcal{Q}_k^d$ for $d = 2$ and $k \in \{5, 6\}$.

Error analysis

Note that

$$|\mathcal{I}^d f - \mathcal{Q}_k^d f| \leq \|\mathcal{I}^d - \mathcal{Q}_k^d\| \|f\|_{H^r(\Omega)}.$$

We can estimate the worst case error of the Smolyak quadrature rule $\mathcal{Q}_k^d$ by bounding the operator norm of $\mathcal{I}^d - \mathcal{Q}_k^d$.

It is known from classical approximation theory that the sequence of univariate CC rules satisfy

$$\|\mathcal{I}^1 - U_k\| \leq \gamma_r 2^{-rk} \tag{4}$$

for some sequence of numbers $(\gamma_r)_{r\geq 0}$.

Lemma

The Smolyak–Clenshaw–Curtis quadrature rules satisfy the bound

$$\|\mathcal{I}^d - \mathcal{Q}_k^d\| \leq \gamma_r \max\{2^{r+1}, \gamma_r(1+2^r)\}^{d-1}\binom{k}{d-1}2^{-rk}.$$

Proof. By dimension-wise induction. The case $d = 1$ is immediate since (4) and the telescoping property imply that

$$\|\mathcal{I}^1 - \mathcal{Q}_k^1\| = \|\mathcal{I}^1 - U_k\| \leq \gamma_r 2^{-rk} \leq \gamma_r \underbrace{\max\{2^{r+1}, \gamma_r(1+2^r)\}}_{\geq 1}\underbrace{\binom{k}{1-1}}_{=1}2^{-rk}$$

as desired.

Next assume that the claim

$$\|\mathcal{I}^d - \mathcal{Q}_k^d\| \le \gamma_r \max\{2^{r+1}, \gamma_r(1+2^r)\}^{d-1} \binom{k}{d-1} 2^{-rk}$$

holds for some $d \ge 1$. Then

$$\begin{aligned}
\mathcal{I}^{d+1} - \mathcal{Q}_{k+1}^{d+1} &= \mathcal{I}^d \otimes \mathcal{I}^1 - \mathcal{Q}_k^d \otimes \mathcal{I}^1 + \mathcal{Q}_k^d \otimes \mathcal{I}^1 - \mathcal{Q}_{k+1}^{d+1} \\
&= (\mathcal{I}^d - \mathcal{Q}_k^d) \otimes \mathcal{I}^1 + \sum_{\substack{|\alpha|_1 \le k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} \left(\bigotimes_{i=1}^d \Delta_{\alpha_i} \right) \otimes \mathcal{I}^1 - \sum_{\substack{|\alpha|_1 \le k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} \left(\bigotimes_{i=1}^d \Delta_{\alpha_i} \right) \otimes U_{k+1-|\alpha|_1} \\
&= (\mathcal{I}^d - \mathcal{Q}_k^d) \otimes \mathcal{I}^1 + \sum_{\substack{|\alpha|_1 \le k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} \left(\bigotimes_{i=1}^d \Delta_{\alpha_i} \right) \otimes (\mathcal{I}^1 - U_{k+1-|\alpha|_1}).
\end{aligned}$$

Taking the operator norm

$$\|\mathcal{I}^{d+1} - \mathcal{Q}_{k+1}^{d+1}\| \le \|\mathcal{I}^d - \mathcal{Q}_k^d\| \|\mathcal{I}^1\| + \sum_{\substack{|\alpha|_1 \le k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} \left(\prod_{i=1}^d \|\Delta_{\alpha_i}\| \right) \|\mathcal{I}^1 - U_{k+1-|\alpha|_1}\|.$$

Here we have $\|\mathcal{I}^1\| = 2$, $\|\mathcal{I}^1 - U_{k+1-|\alpha|_1}\| \le \gamma_r 2^{-r(k+1-|\alpha|_1)}$, and $\|\mathcal{I}^d - \mathcal{Q}_k^d\| \le \gamma_r \max\{2^{r+1}, \gamma_r(1+2^r)\}^{d-1}\binom{k}{d-1}2^{-rk}$ by the induction assumption. Noting that

$$\|\Delta_{\alpha_i}\| \le \|U_{\alpha_i} - \mathcal{I}^1\| + \|\mathcal{I}^1 - U_{\alpha_i - 1}\| \le \gamma_r 2^{-r\alpha_i} + \gamma_r 2^{-r\alpha_i + r} = \gamma_r 2^{-r\alpha_i}(1+2^r)$$

we obtain

$$\sum_{\substack{|\alpha|_1 \le k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} \underbrace{\left(\prod_{i=1}^d \|\Delta_{\alpha_i}\|\right)}_{\le \gamma_r^d 2^{-r|\alpha|_1}(1+2^r)^d} \underbrace{\|\mathcal{I}^1 - U_{k+1-|\alpha|_1}\|}_{\le \gamma_r 2^{-r(k+1-|\alpha|_1)}} \le \sum_{\substack{|\alpha|_1 \le k \\ \alpha \in \mathbb{N}^d,\ \alpha \ge \mathbf{1}}} \gamma_r^{d+1} 2^{-r(k+1)}(1+2^r)^d$$

$$= \binom{k}{d}\gamma_r^{d+1}2^{-r(k+1)}(1+2^r)^d.$$

Hence

$$\|\mathcal{I}^{d+1} - \mathcal{Q}_{k+1}^{d+1}\| \leq \|\mathcal{I}^d - \mathcal{Q}_k^d\| \|\mathcal{I}^1\| + \sum_{\substack{|\alpha|_1 \leq k \\ \alpha \in \mathbb{N}^d,\ \alpha \geq \mathbf{1}}} \left(\prod_{i=1}^d \|\Delta_{\alpha_i}\| \right) \|\mathcal{I}^1 - U_{k+1-|\alpha|_1}\|$$

$$\leq 2\gamma_r \max\{2^{r+1}, \gamma_r(1+2^r)\}^{d-1} \binom{k}{d-1} 2^{-rk} + \gamma_r[\gamma_r(1+2^r)]^d \binom{k}{d} 2^{-r(k+1)}$$

$$\leq 2^{r+1}\gamma_r \max\{2^{r+1}, \gamma_r(1+2^r)\}^{d-1} \binom{k}{d-1} 2^{-r(k+1)} + \gamma_r[\gamma_r(1+2^r)]^d \binom{k}{d} 2^{-r(k+1)}$$

$$\overset{(*)}{\leq} \gamma_r \max\{2^{r+1}, \gamma_r(1+2^r)\}^d 2^{-r(k+1)} \left[\binom{k}{d-1} + \binom{k}{d} \right] \qquad \text{(Pascal's identity)}$$

$$= \gamma_r \max\{2^{r+1}, \gamma_r(1+2^r)\}^d 2^{-r(k+1)} \binom{k+1}{d}$$

proving the assertion. □

(∗) Note that here $x \max\{x, y\}^{d-1} \leq \max\{x, y\}^d$ for $x, y \geq 0$.

A corollary to the previous Lemma is Smolyak's original estimate

$$\|\mathcal{I}^d - \mathcal{Q}_k^d\| \leq Ck^{d-1}2^{-rk},$$

where the constant $C > 0$ depends on r and d.

One can relate this error bound (depending on the level k) to the number of evaluation points $N = N(k,d)$ of the Smolyak–Clenshaw–Curtis rule $\mathcal{Q}_k^d$. Recalling that the CC rules are nested, we get (cf. (3))

$$N \leq \sum_{\substack{|\alpha|_1 = k \\ \alpha \in \mathbb{N}^d,\ \alpha \geq \mathbf{1}}} m_{\alpha_1} \cdots m_{\alpha_d} \leq \sum_{\substack{|\alpha|_1 = k \\ \alpha \in \mathbb{N}^d,\ \alpha \geq \mathbf{1}}} 2^{|\alpha|_1} = 2^k \sum_{\substack{|\alpha|_1 = k \\ \alpha \in \mathbb{N}^d,\ \alpha \geq \mathbf{1}}} 1$$
$$= 2^k \binom{k-1}{d-1} \leq C' 2^k k^{d-1},$$

where $C' > 0$ is a constant that depends on d and we used $m_i \leq 2^i$ as well as the Lemma on slide 9.

For simplicity, let us write $a \lesssim b$ if $a \leq Cb$ for some constant $C > 0$.

Since $N \lesssim 2^k k^{d-1}$, we have $2^{-k} \lesssim \frac{k^{d-1}}{N}$.

Hence, the Smolyak error term can be recast as

$$\|\mathcal{I}^d - \mathcal{Q}_k^d\| \lesssim 2^{-rk} k^{d-1} \lesssim \frac{k^{r(d-1)}}{N^r} k^{d-1} = \frac{k^{(r+1)(d-1)}}{N^r}.$$

For sufficiently large k, we have $2^k \leq N$ and hence $k \leq \log N$; therefore

$$\|\mathcal{I}^d - \mathcal{Q}_k^d\| \lesssim \frac{(\log N)^{(r+1)(d-1)}}{N^r},$$

where the implied coefficient depends on r and d. Hence, for fixed regularity r and fixed d, the method converges at the above rate as $N \to \infty$.

Polynomial exactness

$$\mathbb{P}_k^d = \left\{ \mathbb{R}^d \ni x \mapsto \sum_{\substack{|\beta|_1 \le k \\ \beta \in \mathbb{N}^d}} a_\beta x^\beta \in \mathbb{R};\ a_\beta \in \mathbb{R} \text{ for all } \beta \in \mathbb{N}^d \right\}.$$

$$\bigotimes_{i=1}^d \mathbb{P}_{m_i}^1 = \left\{ \mathbb{R}^d \ni (x_1, \ldots, x_d) \mapsto \prod_{i=1}^d p_i(x_i) \in \mathbb{R};\ p_i \in \mathbb{P}_{m_i}^1 \text{ for } i = 1, \ldots, d \right\}.$$

Lemma

The Smolyak–Clenshaw–Curtis rules satisfy $\mathcal{Q}_k^d f = \mathcal{I}^d f$ for all polynomials

$$f \in \sum_{\substack{|\alpha|_1 = k \\ \alpha \in \mathbb{N}^d}} \mathbb{P}_{m_{\alpha_1}} \otimes \cdots \otimes \mathbb{P}_{m_{\alpha_d}}.$$

Proof. By dimension-wise induction. For $d = 1$, the claim is reduced into

$$\mathcal{I}^1 f = U_k f$$

for all $f \in \Pi_k$. This is true since the CC rule is interpolatory.

Suppose that the claim is true for some $d \geq 1$.

Let $\beta \in \mathbb{N}^{d+1}$ such that $|\beta|_1 = k$ and $k \geq d+1$. Define $f(x_1, \dots, x_{d+1}) = g(x_1, \dots, x_d) f_{d+1}(x_{d+1})$, where $g(x_1, \dots, x_d) = f_1(x_1) \cdots f_d(x_d)$ and $f_i \in \mathbb{P}^1_{m_i}$ for $i = 1, \dots, d+1$. Now clearly $f \in \bigotimes_{i=1}^{d+1} \mathbb{P}^1_{m_{\beta_i}}$. It is sufficient to prove the claim for the function f since linearity of the Smolyak rule implies that the claim then holds for any element in $\sum_{\substack{|\alpha|_1 = k \\ \alpha \in \mathbb{N}^{d+1}}} \bigotimes_{i=1}^{d+1} \mathbb{P}^1_{m_{\alpha_i}}$ as well.

Using dimension recursion and the product structure of f we get

$$\mathcal{Q}_k^{d+1} f = \sum_{i=d}^{k-1} \mathcal{Q}_i^d \otimes \Delta_{k-i} f = \sum_{i=d}^{k-1} \mathcal{Q}_i^d g \cdot \Delta_{k-i} f_{d+1}.$$

If $\beta_{d+1} \leq k - i - 1$, then $m_{\beta_{d+1}} \leq m_{k-i-1} \leq m_{k-i}$ and we have $U_{k-i} f_{d+1} = U_{k-i-1} f_{d+1} = \mathcal{I}^1 f_{d+1}$. Especially $\Delta_{k-i} f_{d+1} = 0$ and we can truncate the expression for $\mathcal{Q}_k^{d+1}$ by considering summation over the indices $k - \beta_{d+1} \leq i \leq k-1$.

Using the fact that $k = |\beta|_1$ allows us to write the rule $\mathcal{Q}_k^{d+1}$ in the form

$$\mathcal{Q}_k^{d+1} f = \sum_{i=\beta_1+\cdots+\beta_d}^{k-1} \mathcal{Q}_i^d g \cdot \Delta_{k-i} f_{d+1}.$$

Our induction hypothesis implies that $\mathcal{I}^d g = \mathcal{Q}_i^d g$ for $\beta_1 + \cdots + \beta_d \leq i \leq k-1$ and we achieve

$$\begin{aligned} \mathcal{Q}_k^{d+1} f &= \sum_{i=\beta_1+\ldots+\beta_d}^{k-1} \mathcal{I}^d g \cdot \Delta_{k-i} f_{d+1} \\ &= \mathcal{I}^d g \cdot U_{k-\beta_1-\cdots-\beta_d} f_{d+1} \\ &= \mathcal{I}^d g \cdot U_{\beta_{d+1}} f_{d+1} \\ &= \mathcal{I}^d g \cdot \mathcal{I}^1 f_{d+1} = \mathcal{I}^{d+1} f \end{aligned}$$

proving the claim. □

Relating the polynomial exactness to the total degree m of "classical" polynomial spaces $\mathbb{P}_m^d$ is rather technical – the explicit expression for the total degree m of exactness in terms of the dimension d and level k of a Smolyak–Clenshaw–Curtis rule $\mathcal{Q}_k^d$ is somewhat complicated, and can be found in [Novak & Ritter (1999)].

The following (weaker) assertion, however, is true for Smolyak–Clenshaw–Curtis rules.

Theorem (Corollary 1 in [Novak & Ritter (1999)])

The Smolyak–Clenshaw–Curtis rule has (at least) a degree $2(k-d)+1$ *of exactness.*

Discussion

During these past two lectures, we have considered the construction and approximation properties of classical, isotropic Smolyak quadrature rules

$$\mathcal{Q}_k^d = \sum_{\substack{|\alpha|_1 \leq k \\ \alpha \in \mathbb{N}^d}} \bigotimes_{i=1}^{d} \Delta_{\alpha_i}.$$

We have seen that

- there exists a computationally useful "combination method" that can be used to effectively implement the isotropic Smolyak rule.
- the Smolyak–Clenshaw–Curtis rule has an error rate

  $$\mathcal{O}\left(\frac{(\log N)^{(d-1)(r+1)}}{N^r}\right)$$

  for functions $f \in H^r([-1,1]^s)$.
- the Smolyak–Clenshaw–Curtis rule is exact for polynomials of total degree (at least) $2(k-d)+1$.

Extensions

In practice, many of these approximation results extend to other, more general quadrature rules

$$\tilde{U}_k^{(j)} f = \sum_{i=1}^{m_k^{(j)}} w_i f(x_i) \approx \int_{\mathcal{I}_j} W_j(x) f(x) \, \mathrm{d}x, \tag{5}$$

with different pairings of intervals $\mathcal{I}_j \subseteq \mathbb{R}$ and weight functions $W_j(x) \geq 0$ (with finite moments). In this case, the Smolyak construction approximates integrals of the form

$$\int_{\mathcal{I}_1 \times \cdots \times \mathcal{I}_d} W_1(x_1) \cdots W_d(x_d) f(x_1, \ldots, x_d) \, \mathrm{d}x_1 \cdots \mathrm{d}x_d.$$

Similar results on convergence and polynomial approximation can be obtained as long as the univariate rules (5) are interpolatory and the sequence $(m_i^{(j)})_{i=1}^{\infty}$ is imposed a sufficient growth condition. It is generally more economical to use nested univariate formulae.

Other extensions

Depending on the application, one may be interested to consider generalized sparse grid constructions

$$\sum_{\alpha \in \mathcal{I}} \bigotimes_{i=1}^{d} (A_{\alpha_i} - A_{\alpha_i - 1}).$$

- The operators $(A_i)_{i=1}^{\infty}$ can be replaced, e.g., by interpolation operators or projection operators. Note that the convergence rates may differ from the quadrature setting!
- In many situations, the components of your function may have different, relative importance or *anisotropy*. For example, x_1 affects the integration problem more than x_2, x_2 affects the result more than x_3, etc. The index set $\mathcal{I}$ can therefore be either tailored to fit the *a priori* information of your problem, or one can use a dimension-adaptive scheme. The combination method (2) no longer works!

These approaches will be featured in the upcoming talks!

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