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Smolyak cubature of given polynomial degree with few nodes for increasing dimension *

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Summary. Some recent investigations (see e.g., Gerstner and Griebel [5], Novak and Ritter [9] and [10], Novak, Ritter and Steinbauer [11], Wasilkowski and Woźniakowski [18] or Petras [13]) show that the so-called Smolyak algorithm applied to a cubature problem on the d-dimensional cube seems to be particularly useful for smooth integrands. The problem is still that the numbers of nodes grow (polynomially but) fast for increasing dimensions. We therefore investigate how to obtain Smolyak cubature formulae with a given degree of polynomial exactness and the asymptotically minimal number of nodes for increasing dimension d and obtain their characterization for a subset of Smolyak formulae. Error bounds and numerical examples show their good behaviour for smooth integrands. A modification can be applied successfully to problems of mathematical finance as indicated by a further numerical example.

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1 Introduction

The Smolyak algorithm is a procedure that derives numerical methods for tensor product problems from those for univariate ones. Here, we consider the numerical calculation of

$$(1) \qquad I^d[f] = \int_{[0,1]^d} f(\mathbf{x})\, d\mathbf{x}, \qquad \mathbf{x} = (x_1, \ldots, x_d).$$

Let therefore be $\mathbf{Q} = Q^{(1)}, Q^{(2)}, \ldots$ a sequence of quadrature formulae

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$$Q^{(i)}[f] := Q_{n_i}[f] := \sum_{\nu=1}^{n_i} a_\nu^{(i)} f(x_\nu^{(i)}) = \int_0^1 f(x)\,dx - R^{(i)}[f], \qquad x_\nu^{(i)} \in [0,1] \tag{2}$$

where $R^{(i)}$ is the residual of $Q^{(i)}$. The corresponding *k-stage Smolyak formulae* (cf. Smolyak [16]) to the *basic sequence* $\mathbf{Q}$ for numerical calculation of $I^d[f]$ are now given by

$$Q(d+k,d) = \sum_{k+1\le|\mathbf{i}|\le d+k} (-1)^{d+k-|\mathbf{i}|} \binom{d-1}{|\mathbf{i}|-k-1} \times Q^{(i_1)} \otimes \ldots \otimes Q^{(i_d)}, \tag{3}$$

where

$$Q^{(0)}[f] = 0, \qquad \mathbf{i} = (i_1, \ldots, i_d) \ge (0, \ldots, 0) \qquad \text{and} \qquad |\mathbf{i}| = \sum_{\nu=1}^{d} i_\nu \tag{4}$$

as well as

$$Q^{(i_1)} \otimes \ldots \otimes Q^{(i_d)}[f] = \sum_{\nu_1=1}^{n_1} \cdots \sum_{\nu_d=1}^{n_d} a_{\nu_1}^{(i_1)} \cdots a_{\nu_d}^{(i_d)} \cdot f(x_{\nu_1}^{(i_1)}, \ldots, x_{\nu_1}^{(i_d)}). \tag{5}$$

Another way of writing Smolyak cubature is to set $Q^{(0)} = 0$,

$$\Delta^{(i)} = \begin{cases} Q^{(i)} - Q^{(i-1)} & \text{for } i > 0 \\ 0 & \text{otherwise} \end{cases} \qquad \text{and} \qquad Q(d+k,d) = \sum_{|\mathbf{i}|\le d+k} \Delta^{(i_1)} \otimes \ldots \otimes \Delta^{(i_d)} \tag{6}$$

(for further properties, see, e.g., Novak and Ritter [10] or Wasilkowski and Woźniakowski [18]). The cubature error is defined by

$$R(d+k,d)[f] = I^d[f] - Q(d+k,d)[f]. \tag{7}$$

Some competitors of the Smolyak algorithms are, e.g.

1. Product formulae (see (5))
2. Monte-Carlo formulae (see Caflisch [2] and Niederreiter [8])
3. Quasi-Monte-Carlo formulae (see Caflisch [2] and Niederreiter [8])
4. Lattice rules (see Sloan and Joe [14])
5. The fully symmetric rules of Genz [4].

Some remarks concerning these formulae, respectively, are:

1. The numbers of nodes of nontrivial product formulae increase exponentially with increasing dimension.
2. The Monte-Carlo method is – in a stochastic sense – a rather robust method but the convergence rate of a "pure" Monte-Carlo method is rather poor.
3. Quasi-Monte-Carlo rules have (like the trapezoidal rule for univariate integration) favourable properties for integrands with low-order smoothness but if higher order derivatives of the integrand exist, the known rules do not use the full smoothness.
4. Lattice rules are particularly designed for the integration of periodic functions. If we want to obtain a high convergence rate when applying them to smooth non-periodic functions, we have to transform the integrand into a periodic function. These transformations often reduce the smoothness and increase norms of derivatives drastically.
5. Novak and Ritter [10] noticed that the Genz rules can be interpreted as Smolyak rules.

In the recent literature on cubature of non-periodic functions with Smolyak's algorithm, mainly two basic sequences have been investigated:

1. **The Clenshaw-Curtis sequence:** $Q^{(1)}[f] = f(1/2)$ and $Q^{(i)}$, $i = 2, 3, \ldots$ is the $2^{\mathrm{i}-1} + 1$-point Clenshaw-Curtis formula (see Brass [1] or Novak and Ritter [9]) transformed to $[0, 1]$. We denote the resulting Smolyak formulae by Q^{CC}.
2. **The Kronrod-Patterson sequence:** $Q^{(1)}[f] = f(1/2)$, $Q^{(2)}$ is the 3-point Gaussian formula and $Q^{(i)}$, $i = 3, \ldots, 9$, are the successive $2^i - 1$-point Kronrod-Patterson extensions (see Patterson [12] or Gerstner and Griebel [5]) transformed to $[0, 1]$. We denote the resulting Smolyak formulae by Q^{KP}.

The second sequence has the advantage that the polynomial degree of exactness of the respective formulae is considerably higher, while a disadvantage is that the numbers of nodes increase faster.

The properties of the Smolyak cubature formulae of course depend on those of the underlying quadrature formulae. We therefore introduce some notations and notions concerning these quadrature formulae.

Definition 1 *A quadrature formula $Q^{(i)}$ is called positive if all its coefficients $a_\nu^{(i)}$ (see (2)) are nonnegative. We say that the basic sequence $\mathbf{Q}$ is positive if all its quadrature formulae are positive. The number of nodes is denoted by $n(Q^{(i)})$ for quadrature and by $n(d + k, d) := n(Q(d + k, d))$ for Smolyak formulae. The degree of a quadrature or cubature formula is*

$$\deg(Q^{(i)}) = \sup\{s \mid R^{(i)}[\mathbb{P}_s] = \{0\}\} \quad \textit{or}$$

$$\deg(Q(d+k,d)) = \sup\{s \mid R(d+k,d)[\mathbb{P}_s^{(d)}] = \{0\}\} \tag{8}$$

respectively ($\mathbb{P}_s^{(d)}$ denotes the d-variate polynomials of total degree less than $s+1$). We call $Q^{(i+1)}$ extension of $Q^{(i)}$ and denote by δ_i the number of nodes used by $Q^{(i+1)}$ but not by $Q^{(i)}$ (i.e., in particular, $\delta_0 = n(Q^{(1)})$). If $\delta_1 = \ldots = \delta_m = 0 \neq \delta_{m+1}$, we say that $\mathbf{Q}$ *is m-degenerate. A 0-degenerate sequence will be called regular and we carry the notion of regularity and degeneracy over to the corresponding Smolyak formulae. Finally, we denote by $()^i$ the function p given by $p(x) = x^i$.*

In particular for high dimensions, the number of nodes increase fast with the number of stages and for a given number of stages, the number of nodes increase fast with the dimension. Therefore, we want to investigate Smolyak formulae of given degree using relatively few nodes. At the same time we want to achieve good error properties. It was pointed out in [13] that a high algebraic degree $\deg(Q(d+k,d))$ implies in a certain sense a small error for smooth functions. The main tool will be the repetition of quadrature formulae in the basic sequence. We call formulae with such a repetition "delay Smolyak formulae".

The number $n(d+k,d)$ of nodes used by the Smolyak formula $Q(d+k,d)$ can be calculated iteratively from the number of nodes of the elements of the basic sequence of quadrature formulae. Namely,

$$n(d+k+1,d+1) = \delta_0 \cdot n(d+k,d) + \sum_{\nu=1}^{k} \delta_\nu \cdot n(d+k-\nu,d),$$

$$n(1+k,1) = n(Q^{(k+1)}) \tag{9}$$

(see [13, Sect. 3]). By a more explicit formulae that will be proved below, we will see later how the numbers of nodes for fixed k and increasing d grow polynomially if $n(1,1) = \delta_0 = 1$ i.e., if $Q^{(1)}$ is based on one node and exponentially if $\delta_0 > 1$.

It is the purpose of this paper to characterize and derive methods of a given algebraic degree of precision using the minimal number of nodes if d increases. This means that we try to retain the favourable properties of the Smolyak algorithm for smooth functions with the asymptotically minimal effort. For this purpose, we derive an expression for the number of nodes of a Smolyak formula in Sect. 2. In Sect. 3, we characterize regularly asymptotical minimal Smolyak formulae and give examples in Sect. 4 and recommend a certain positive basic sequence. Then, in Sect. 5 and 6, we give numerical tests including an example from finance for high dimensional integration in weighted tensor product spaces, i.e., in spaces, where the dimensions are of different importance. Finally, in Sect. 7, we discuss briefly some properties of degenerate Smolyak cubature.

2 The number of nodes

The number of nodes used by $Q(d+k,d)$ can be calculated by formula (9). Of course, in our approach, it may happen by chance that some weights a_ν in the representation

$$(13) \qquad Q(d+k,d)[f] = \sum_{\nu=1}^{n} a_\nu f(\mathbf{x}_\nu), \qquad \mathbf{x}_\nu = (x_{\nu,1},\ldots,x_{\nu,d})$$

vanish. In this special case, which seems to be hard to predict by considering the underlying basic sequence $\left(Q^{(i)}\right)_{i\in\mathbb{N}}$, we still count the corresponding node. In our double precision numerical computations, it never occurred that a coefficient a_ν has been of modulus less than 10^{-7}.

Now, everything depends on the sequence $\left(Q^{(i)}\right)_{i\in\mathbb{N}}$, respectively on the sequence $\left(\delta_i\right)_{i\in\mathbb{N}}$. Instead of calculating $n(d+k,d)$ for each pair (k,d), we give a general formula holding for all d, in which all coefficients can be calculated for given fixed k.

Theorem 1 *The number $n(d+k,d)$ of nodes of the Smolyak formula $Q(d+k,d)$ is given by*

$$(14) \qquad n(d+k,d) = \delta_0^d \sum_{j=0}^{k} c_{j,k} \binom{d}{j}, \qquad \textit{where } \binom{d}{j} := 0 \textit{ if } j > d,$$

$$(15) \qquad c_{j,k} = \sum_{\nu=1}^{k-j+1} \frac{\delta_\nu}{\delta_0} c_{j-1,k-\nu}, \qquad j = 1,\ldots,k$$

and

$$(16) \qquad c_{0,k} = 1.$$

Lemma 1 *Formula (14) holds with*

$$(17) \qquad c_{j,k} = (-1)^{j+1} \left\{ \sum_{\mu=j+1}^{k} (-1)^\mu c_{\mu,k} + \sum_{\nu=1}^{k-j+1} \frac{\delta_\nu}{\delta_0} \sum_{\mu=j-1}^{k-\nu} (-1)^\mu c_{\mu,k-\nu} \right\}, \qquad j = 1,\ldots,k,$$

and

$$(18) \qquad c_{0,k} = \frac{n(1+k,1)}{\delta_0} - c_{1,k}.$$

Proof. This is proved by induction over the dimension. The case $d = 1$ in (14) reads $n(1+k,1) = \delta_0(c_{0,k} + c_{1,k})$, which is equation (18). Suppose therefore, the lemma is proved for dimensions less than d. By formula (9) and by

$$\binom{d-1}{\mu} = \sum_{i=0}^{\mu} (-1)^{\mu-i} \binom{d}{i} \tag{19}$$

(see Gradshteyn and Ryzhik [6, eq. 0.1514]), we obtain

$$\begin{aligned}
\frac{n(k+d,d)}{\delta_0^d} &= \sum_{\nu=0}^{k} \frac{\delta_\nu}{\delta_0^d} n(d-1+k-\nu, d-1) \\
&= \sum_{\nu=0}^{k} \frac{\delta_\nu}{\delta_0} \sum_{\mu=0}^{k-\nu} c_{\mu,k-\nu} \binom{d-1}{\mu} \\
&= \sum_{\mu=0}^{k} \binom{d-1}{\mu} \sum_{\nu=0}^{k-\mu} \frac{\delta_\nu}{\delta_0} c_{\mu,k-\nu} \\
&= \sum_{\mu=0}^{k} \sum_{i=0}^{\mu} (-1)^{\mu-i} \binom{d}{i} \sum_{\nu=0}^{k-\mu} \frac{\delta_\nu}{\delta_0} c_{\mu,k-\nu} \\
&= \sum_{i=0}^{k} \binom{d}{i} \left\{ \sum_{\nu=0}^{k-i} \frac{\delta_\nu}{\delta_0} \sum_{\mu=i}^{k-\nu} (-1)^{\mathrm{i}+\mu} c_{\mu,k-\nu} \right\}. \qquad (20)
\end{aligned}$$

Comparing coefficients, we have

$$\begin{aligned}
c_{i,k} &= \sum_{\nu=0}^{k-i} \frac{\delta_\nu}{\delta_0} \sum_{\mu=i}^{k-\nu} (-1)^{\mathrm{i}+\mu} c_{\mu,k-\nu} \\
&= c_{i,k} - c_{i+1,k} + \sum_{\mu=i+2}^{k} (-1)^{\mathrm{i}+\mu} c_{\mu,k} \\
&\quad + \sum_{\nu=1}^{k-i} \frac{\delta_\nu}{\delta_0} \sum_{\mu=i}^{k-\nu} (-1)^{\mathrm{i}+\mu} c_{\mu,k-\nu}. \qquad (21)
\end{aligned}$$

We set $i + 1 = j$ and obtain the lemma. □

Proof of Theorem. The theorem is equivalent to Lemma 1 at least for $j = k$. Suppose, the result is true for $c_{k,k}, c_{k-1,k}, \ldots, c_{j+1,k}$. Then, we insert this in the first sum of the right-hand side of (17) in Lemma 1 and obtain

$$
\begin{aligned}
c_{j,k} &= (-1)^{j+1}\left\{\sum_{\mu=j+1}^{k}(-1)^{\mu}\sum_{\nu=1}^{k-\mu+1}\frac{\delta_\nu}{\delta_0}c_{\mu-1,k-\nu}\right.\\
&\qquad\left.+\sum_{\mu=j-1}^{k-1}(-1)^{\mu}\sum_{\nu=1}^{k-\mu}\frac{\delta_\nu}{\delta_0}c_{\mu,k-\nu}\right\}\\
&= (-1)^{j+1}\left\{\sum_{\mu=j+1}^{k}(-1)^{\mu}\sum_{\nu=1}^{k-\mu+1}\frac{\delta_\nu}{\delta_0}c_{\mu-1,k-\nu}\right.\\
&\qquad\left.+\sum_{\mu=j}^{k}(-1)^{\mu+1}\sum_{\nu=1}^{k-\mu+1}\frac{\delta_\nu}{\delta_0}c_{\mu-1,k-\nu}\right\}\\
&= \sum_{\nu=1}^{k-j+1}\frac{\delta_\nu}{\delta_0}c_{j-1,k-\nu}, \qquad (22)
\end{aligned}
$$

which is (15). We still have to prove formula (16), which obviously holds for $k=0$, i.e., for product formulae. Suppose now, it holds for $k=0,1,\ldots,s-1$. Then, by (18) and (15),

$$
c_{0,s} = \frac{n(1+s,1)}{\delta_0} - c_{1,s} = \frac{1}{\delta_0}\sum_{\nu=0}^{s}\delta_\nu - \sum_{\nu=1}^{s}\frac{\delta_\nu}{\delta_0}c_{0,s-\nu} = \frac{\delta_0}{\delta_0} = 1. \qquad (23)
$$

□

3 Minimality conditions

Definition 2 *Let* **Q** *be a basic sequence satisfying*

$$
\deg(Q(d+k(d),d)) \geq s \qquad (24)
$$

for all d. Then, we say that **Q** *is asymptotically minimal (and write a.m.) for degree s if for each basic sequence* $\widetilde{\mathbf{Q}}$*, the corresponding Smolyak formulae of algebraic degree $\geq s$ use less nodes than $Q(d+k(d),d)$ for at most finitely many dimensions. We call a positive basic sequence* **Q** *p-asymptotically minimal (p-a.m.), if it is a.m. among all positive basic sequences. A regular basic sequence is called regularly (p-)a.m. if it is (p-).a.m. among all regular basic sequences.*

Note that we allow variation in the number of stages, i.e., we allow k to depend on d, in order to achieve a certain degree. It will turn out that there are already regularly asymptotically minimal sequences using a fixed k for all d although they compete with sequences where a varying $k = k(d)$ is allowed.

Completely analogous as in Novak and Ritter [10], we obtain

Proposition 1 *If* $\deg(Q^{(i)}) \geq 2i - 1$ *for all* i*, then,*

$$\deg(Q(d+k,d)) \geq 2k+1. \tag{25}$$

We might hope that the condition of Proposition 1 is also necessary. However, this is not true – things are more complicated.

Proposition 1 was originally proved by Novak and Ritter for a specific basic sequence. Many basic sequences (of positive quadrature formulae) satisfy the assumptions of this proposition and the number of nodes used by the corresponding Smolyak formulae increases only polynomially as a function of the dimension d. If $n(Q^{(1)}) > 1$, then the number of nodes used by $Q(d+k,d)$ increases exponentially and the corresponding basic sequence cannot be (p-) asymptotically minimal. If $n(Q^{(1)}) = 1$ and $\delta_1 > 0$, then the polynomial increase is of degree k with main coefficient $(\delta_1/\delta_0)^k$. Hence, we have

Corollary 1 *A regular basic sequence with* $n(Q^{(1)}) > 1$ *cannot be (p-)a.m. Furthermore, a regular (p-)a.m. basic sequence for degree* $2k+1$ *can have at most* k *stages for almost all dimensions.*

In fact, we will first consider only regular basic sequences, i.e., those with $\delta_1 \neq 0$. In Sect. 7, we discuss briefly the degenerate case.

In this section, we prove two theorems. The first one concerns the problem, which regular Smolyak formulae have a certain degree of exactness for infinitely many dimensions. It is the counterpart of Proposition 1. Theorem 3a/b give conditions for regular (p-) asymptotic minimality.

Theorem 2 *Let* $\mathbf{Q}$ *be a regular basic sequence satisfying* $n(Q^{(1)}) = 1$*, let* $k \leq s$ *be fixed and let* $\deg Q(d+k,d) \geq 2s+1$ *for more than* $s+1$ *dimensions d. Then,* $k = s$ *and*

1. *if s is odd,* $\mathbf{Q}$ *satisfies* $\deg(Q^{(i)}) \geq 2i - 1$ *for* $i = 1, \ldots, s+1$*,*
2. *if s is even and* $\mathbf{Q}$ *is positive, then* $\deg(Q^{(i)}) \geq 2i-1$ *for* $i = 1, \ldots, s+1$ *and*
3. *if s is even, we have*
   (a) $Q^{(1)}[f] = f(1/2)$*,*
   (b) $R^{(i)}[()^0] = R^{(i)}[()^1] = 0$ *for all* i *and*
   (c) either $\deg(Q^{(i)}) \geq 2i-1$ *or the sequence* $R^{(2)}[()^2], \ldots, R^{(s+1)}[()^2]$ *is uniquely determined with* $R^{(2)}[()^2] = 1/6$*.*

Theorem 2 distinguishes essentially two cases, namely if $\deg(Q^{(2)}) \geq 2$ or not. The second case is much more complicated and causes some problems in the following.

Theorem 3a *The regular positive sequence* $Q^{(1)}, \dots, Q^{(k+1)}$ *is regularly p-a.m. for degree* $2k+1$ *if and only if*

1. $Q^{(1)}[f] = f(1/2)$
2. $\deg(Q^{(i)}) \geq 2i - 1$
3. $Q^{(1)}, \dots, Q^{(k)}$ *is regularly p-a.m. for degree* $2k-1$
4. $Q^{(k+1)}$ *is positive and, among all positive extensions of* $Q^{(k)}$ *having degree* $\geq 2k+1$, $Q^{(k+1)}$ *has minimal number of additional nodes.*

With the proof of Theorem 3a, we will also have proved

Theorem 3b *The basic sequence* $\mathbf{Q}$ *satisfying* $\deg(Q^{(2)}) \geq 2$ *is regularly a.m. for degree* $2k+1$ *among all basic sequences* $\widetilde{\mathbf{Q}}$ *also satisfying* $\deg(\widetilde{Q}^{(2)}) \geq 2$ *if and only if*

1. $Q^{(1)}[f] = f(1/2)$
2. $\deg(Q^{(i)}) \geq 2i - 1$
3. $Q^{(1)}, \dots, Q^{(k)}$ *is regularly a.m. for degree* $2k-1$ *among all* $\widetilde{\mathbf{Q}}$ *satisfying* $\deg(\widetilde{Q}^{(2)}) \geq 2$
4. *among all extensions of* $Q^{(k)}$ *having degree* $\geq 2k+1$, $Q^{(k+1)}$ *has minimal number of additional nodes.*

For the proofs of the theorems, we need a series of lemmas and corollaries. In all these Lemmas, we will use

Assumption *Throughout this section, we will assume that all basic sequences are regular.*

Representation (6) for Smolyak cubature formulae indicates that the following lemma may be helpful if f is of the form

$$f(\mathbf{x}) = h(x_1) \cdot \ldots \cdot h(x_d) \tag{26}$$

Lemma 2 *Let* $J, \omega_0, \dots, \omega_k \in \mathbb{R}$ *and define*

$$M_s^{(k)} = \sum_{|\mathbf{i}| \leq k} \omega_{i_1} \cdot \ldots \cdot \omega_{i_s}. \qquad \text{and} \qquad \widetilde{M}_s^{(k)} = \sum_{\substack{|\mathbf{i}| \leq k \\ i_\nu \geq 1}} \omega_{i_1} \cdot \ldots \cdot \omega_{i_s}. \tag{27}$$

If $M_\sigma^{(k)} = J^\sigma$ *for* $\sigma = 1, \dots, s-1 \leq k+1$, *then*

$$M_s^{(k)} = \widetilde{M}_s^{(k)} + J^s - (J - \omega_0)^s \tag{28}$$

Proof. The Lemma is obviously true for $s = 1$. We now apply the lemma to $M_\sigma^{(k)}$ and use the assumption:

$$\widetilde{M}_\sigma^{(k)} = M_\sigma^{(k)} - J^\sigma + (J - \omega_0)^\sigma = (J - \omega_0)^\sigma, \qquad \sigma = 1, \dots, s-1. \tag{29}$$

Together with setting $\widetilde{M}_0^{(k)} := 1$ and collecting all terms containing a certain number of factors ω_0, this gives

$$\begin{aligned} M_s^{(k)} &= \sum_{\nu=0}^{k} \binom{s}{\nu} \omega_0^{\nu} \widetilde{M}_{s-\nu}^{(k)} \\ &= \widetilde{M}_s^{(k)} + \sum_{\nu=1}^{s} \binom{s}{\nu} \omega_0^{\nu} (J - \omega_0)^{s-\nu} \\ &= \widetilde{M}_s^{(k)} + \big(\omega_0 + (J - \omega_0)\big)^s - (J - \omega_0)^s. \end{aligned} \tag{30}$$

□

Lemma 3 *If f is of the form (26) and $R(d+k,d)[f] = 0$ for $d = 1, \ldots, s$, then,*

$$\sum_{\substack{|\mathbf{i}| \leq d+k \\ i_\nu \geq 2}} \Delta^{(i_1)}[h] \otimes \ldots \otimes \Delta^{(i_d)}[h] = \left(R^{(1)}[h]\right)^d, \qquad \textit{for} \quad d = 1, \ldots, s. \tag{31}$$

Proof. The corollary is nothing but Lemma 2 applied with $J = I[h]$, $\omega_i = \Delta^{(i+1)}[h]$ and $M_d^{(k)} = Q(d+k,d)[f]$. □

Lemma 4 *Let f be of the form (26) and let $R(d+k,d)[f] = 0$ for $d = 1, \ldots, k+1$. Then, $R^{(1)}[h] = 0$.*

Proof. We can apply Lemma 3 with $s = k+1$. The $k+1$-st equation then reads

$$0 = \left(R^{(1)}[h]\right)^{k+1} \tag{32}$$

because the sum on the left-hand side of (31) is empty. □

Since a 1-point formula can never be exact for $\mathbb{P}_2$ and $Q^{(1)}[f] = f(1/2)$ defines the only 1-point formula of degree 1, Lemma 4 applied to all $h \in \{()^0, ()^1, ()^2\}$ gives

Corollary 2 *Let $\mathbf{Q}$ satisfy $n(Q^{(1)}) = 1$. Then the corresponding k-stage Smolyak formulae cannot have degree $\geq 2k+2$ for all $d = 1, \ldots, k+1$. If the degree is $\geq 2k+1$ for all $d = 1, \ldots, k+1$, then $Q^{(1)}[f] = f(1/2)$.*

The k-th equation in Lemma 3 yields

Corollary 3 *Let f be of the form (26) and let $R(d+k,d)[f] = 0$ for $d = 1,\ldots,k$. Then,*

$$\left(\Delta^{(2)}[h]\right)^k = \left(R^{(1)}[h] - R^{(2)}[h]\right)^k = \left(R^{(1)}[h]\right)^k \tag{33}$$

Lemma 5 *Let $Q^{(1)}[f] = f(1/2)$ and let $R^{(i)}[()^2] = 0$ for all $i \geq 2$. Then,*

$$\begin{aligned} R(1+s,1)[()^2] &= R(2+s,2)[()^2 \otimes ()^2] = \ldots \\ &= R(2s,s)[()^2 \otimes \ldots \otimes ()^2] = 0 \end{aligned} \tag{34}$$

but

$$R(2s+1,s+1)[()^2 \otimes \ldots \otimes ()^2] \neq 0. \tag{35}$$

Proof. The vanishing of the error functionals $R(1+s,1),\ldots R(2s-1,s-1)$ follows from Proposition 1, since the Smolyak formulae act on $()^2 \otimes \ldots \otimes ()^2$ exactly like Smolyak formulae satisfying $Q^{(1)}[f] = f(1/2)$ and $\deg(Q^{(i)}) \geq 2i-1$. If (35) would not hold, then, by Lemma 4, $R^{(1)}[()^2] = 0$, which is not true. □

Lemma 6 *Let $Q^{(1)}[f] = f(1/2)$ and let $\deg(Q(d+k,d)) \geq 2k+1$ for $d = 1,\ldots,k+1$. Let furthermore $i \in \{0,1,\ldots,2k+1\}$ denote the smallest number such that $()^i$ is not integrated exactly by some $Q^{(s)}$ with $i \leq 2s-1$. Then, $i \leq 2$.*

Proof. Let $i > 2$ and let s be the largest number such that $Q^{(s)}$ does not integrate $()^i$ exact. This cannot be $k+1$ since

$$R^{(k+1)}[()^i] = R(1+k,1)[()^i] = 0 \tag{36}$$

by assumption. Define now

$$f(\mathbf{x}) = x_1^i g(x_2,\ldots,x_d), \qquad \text{where } g(x_2,\ldots,x_d) = x_2^2 x_3^2 \ldots x_d^2. \tag{37}$$

Then, the error representation (2) in [13] yields

$$R(d+k,d)[f] = \sum_{\nu=1}^{s+1} \Delta^{(\nu)}[()^i] R(d+k-\nu,d-1)[g]. \tag{38}$$

If $d = k-s+2$, then Lemma 5 yields

$$R(d+k-\nu,d-1)[g] \begin{cases} = 0 & \text{for } \nu \leq s \text{ and} \\ \neq 0 & \text{for } \nu = s+1 \end{cases}. \tag{39}$$

Since $\Delta^{(s+1)}[()^i] = Q^{(s+1)}[()^i] - Q^{(s)}[()^i] = R^{(s)}[()^i] - R^{(s+1)}[()^i] \neq 0$, we have $R(d+k,d)[f] \neq 0$ and therefore a contradiction, since the degree of f is less than or equal to $i + 2(k-s+1) \leq 2k+1$. □

Lemma 7 *Let* $n(Q^{(1)}) = 1$*, let* $\deg(Q(d+k,d)) \geq 2k+1$ *for* $d = 1,\ldots,k$ *and let* $R^{(2)}[()^2] = 0$*, then* $R^{(i)}[()^2] = 0$ *for* $i = 3,\ldots,k+1$.

Proof. Using Corollary 2, the assumptions imply $Q^{(1)}[f] = f(1/2)$ and hence $\Delta^{(2)}[()^2] \neq 0$. Therefore, Corollary 3 and Lemma 3 yield

$$\text{(40)} \qquad \sum_{\substack{|\mathbf{i}|\leq d+k \\ i_\nu \geq 2 \\ \neq (2,2,\ldots,2)}} \Delta^{(i_\nu)}[()^2] = 0, \qquad \text{for } d = 1,\ldots,k-1.$$

$d = k-1$ yields $\Delta^{(3)}[()^2]\Delta^{(2)}[()^2]^{d-1} = 0$, i.e., $\Delta^{(3)}[()^2] = 0$. Plugging this into equation (40) for $d = k-2$ gives $\Delta^{(4)}[()^2]\Delta^{(4)}[()^2]^{d-1} = 0$ i.e., $\Delta^{(4)}[()^2] = 0$ etc. □

Lemma 8 *If* $\deg(Q(d+k,d)) \geq 2k+1$ *for* $d = 1,\ldots,k+1$*, then* $\deg(Q^{(i)}) \geq 1$ *for* $i = 1,\ldots,k+1$.

Proof. Corollary 2 says $\deg(Q^{(1)}) = 1$. The same procedure as in the proof of Lemma 7 applied to $()^0$ and $()^1$ instead of $()^2$ now yields successively $\deg(Q^{(i)}) \geq 1$ for $i = 1,\ldots,k+1$. □

Lemma 9 *If a* k*-stage Smolyak algorithm has order* $\geq 2k+1$ *for more than* k *different dimensions, then all basic formulae integrate constant functions exact.*

Proof. Let $r_\nu := \Delta^{(\nu+1)}[1]$. Then,

$$\text{(41)} \qquad Q(d+k,d)[1] = \sum_{|\mathbf{i}|\leq k} r_{i_1} \otimes \ldots \otimes r_{i_d}.$$

Let $j_\mathbf{i}(\nu)$ be the frequency of the index ν in $\mathbf{i}$ and let $\mathbf{j_i} = \{j_\mathbf{i}(1),\ldots,j_\mathbf{i}(k)\}$ be the frequency set (the frequency of the index 0 need not be mentioned since $\sum_{\nu=0}^{k} j_\mathbf{i}(\nu) = d$). Define $J_\mathbf{i} := j_\mathbf{i}(1) + \ldots + j_\mathbf{i}(k) \leq k$. Each product with frequency set $\mathbf{j_i}$ appears exactly

$$\text{(42)} \qquad s(\mathbf{j_i}, d) := \frac{1}{j_\mathbf{i}(1)! \cdot \ldots \cdot j_\mathbf{i}(k)!} \prod_{\nu=d+1-J_\mathbf{i}}^{d} \nu$$

times, i.e., $s(\mathbf{j_i}, d)$ as a function of d is a polynomial of degree $\leq k$. Note that equation (42) holds also when $J_\mathbf{i} > d$ because then, both sides are zero. With this notation, the quadrature value is now

$$\text{(43)} \qquad Q(d+k,d)[1] = r_0^{d-k} \sum_{J_\mathbf{i}\leq k} s(\mathbf{j_i}, d) r_0^{k-J_\mathbf{i}} \cdot \left(r_2^{j_\mathbf{i}(2)} \cdot \ldots \cdot r_k^{j_\mathbf{i}(k)} \right).$$

This is of the form $r_0^{d-k}p(d)$ with $p \in \mathbb{P}_k$. If $p(x) \not\equiv 1$ or $r_0 \neq 1$, the equation

$$p(d) = r_0^{k-d} =: h(d) \tag{44}$$

can hold for at most $k+1$ different dimensions d. Namely, if $r_0 = 1$ and $p(x) \not\equiv 1$, $p - h$ is in $\mathbb{P}_k$ and nontrivial and can therefore have at most k zeros. Let now $r_0 \neq 1$. If p coincides with h at $k+1$ (or more) points, it is an interpolation polynomial and, since $\operatorname{sign}(h^{(k)})$ is constant, has exactly $k+1$ points with h in common, which follows readily from the classical error representation for the interpolation polynomial (see Conte and de Boor [3, Theorem 4.3]). Hence, we have proved that if $Q(d+k,d)[1]$ is 1 for at least $k+2$ dimensions d, then it is for all d. The first part of Corollary 2 now gives the statement. □

Proof of Theorem 2. By Lemma 9, the assumption yields $\deg(Q(d+k,d)) \geq 2k+1$ for $d = 1,\dots,k+1$. Then, 3b) is already proved by Lemma 8. The equation $s = k$ is now an immediate consequence of Lemma 5.

1. Since k is odd, equation (33) gives $R^{(2)}[()^2] = 0$. Lemma 7 now implies that also $R^{(3)}[()^2] = \ldots = R^{(k+1)}[()^2] = 0$. Applying Lemma 6 gives the result.
2. For even k, since $R^{(i)}[()^0] = R^{(i)}[()^1] = 0$, Corollary 3 gives $R^{(2)}[(\cdot - 1/2)^2] = 1/12 - Q^{(2)}[(\cdot - 1/2)^2] \in \{0, 1/6\}$. If $R^{(2)}[(\cdot - 1/2)^2] = 0$, we can proceed as in the proof of 1.) and obtain the same implication. If $R^{(2)}[(\cdot - 1/2)^2] = 1/6$, we have $Q^{(2)}[(\cdot - 1/2)^2] = -1/12$, i.e., a negative number for a positive integrand, such that $Q^{(2)}$ is not positive.
3. a) and b) have already been proved and the first case in c) is the case $R^{(2)}[(\cdot - 1/2)^2] = 0$ discussed in the proof of 2.). If now $R^{(2)}[(\cdot - 1/2)^2] = 1/6$, we have by b) that $R^{(2)}[(\cdot)^2] = 1/6$. As in the proof of Lemma 7, the equations of Lemma 3 determine successively the values $\Delta^{(\nu)}[()^2]\Delta^{(2)}[()^2]^{d-1}$, $\nu = 3,\dots,k$. Since $R^{(2)}[()^2)] = 1/6$ and $R^{(k+1)}[()^2] = 0$ are known, this determines all $R^{(i)}[()^2]$. □

Proof of Theorem 3a. Each positive formula of degree $2k-1$ can of course be extended to a positive formula of degree $2k+1$. Namely, we can take any positive formula of degree $2k+1$ and say that this is an extension. The necessity of 1.) follows from Theorem 2. By Theorem 1, the coefficient $c_{j,k}$ is monotonically increasing with respect to $\delta_1, \delta_2, \dots, \delta_{k-j+1}$ and $c_{j-1,k-1}, c_{j-1,k-2}, \dots, c_{j-1,j-1}$ and independent of all other δ_ν and $c_{j-1,\nu}$. Repeating this argument, we see that $c_{j,k}$ is only dependent on and monotonically increasing with respect to $\delta_1, \delta_2, \dots, \delta_{k-j+1}$ and $c_{0,k-j} = 1, \dots, c_{0,0} = 1$. We furthermore note that all $c_{j,k}$ are nonnegative. In order that $\{Q^{(1)}, \dots, Q^{(k)}\}$ be regularly a.m. for degree $2k+1$ it is necessary and sufficient that the coefficients δ_ν are minimal for $\nu = 1,\dots,k-1$ and among those, δ_k is also minimal. □

4 Example algorithms

Up to now, we collected quite a lot of theory in order to characterize regularly asymptotically minimal basic sequences. Nevertheless we do not know yet, e.g., how many sequences for a certain degree exist, whether there are positive sequences among them, or if the second case in Theorem 2.3c) may occur. Before answering these questions, at least for certain degrees, we start with defining a positive sequence that is not far from being asymptotically minimal and will be recommended for numerical computations. It is a delayed basic sequence of Kronrod-Patterson formulae:

$$Q^{(i)} = Q_m^{KP}, \qquad \frac{3m+4}{8} \le i \le \frac{3m+3}{4},$$

(45) $$m = 1, 3, 7, 15, 31, \ldots,$$

i.e.,

$$Q^{(1)} = Q_1^{KP}, \quad Q^{(2)} = Q^{(3)} = Q_3^{KP},$$

(46) $$Q^{(4)} = Q^{(5)} = Q^{(6)} = Q_7^{KP}, \ldots$$

Since $\deg(Q_{2^i-1}^{KP}) = 3 \cdot 2^{i-1} - 1$ for $i > 1$ (see Monegato [7]), the corresponding basic sequence satisfies the assumptions of Proposition 1. We denote the corresponding Kronrod-Patterson-Smolyak delay algorithm by Q^{del}

In order to illustrate the effect of the delay, we compare the number of nodes used by Q^{del} with Q^{KP} and Q^{CC} for dimension $d = 10$.

Table 1. $n(10 + k, 10)$

k	3	4	5	6	7	8
Q^{CC}	1581	8801	41265	171425	652065	2320385
Q^{KP}	2001	13441	77505	397825	1862145	8085505
Q^{del}	1201	5281	19105	60225	169185	434145

Figures 1 and 2 give a comparison between the nodes of the two 321-point formula $Q^{del}(16, 2)$ and $Q^{CC}(8, 2)$.

Theorem 4 *Let k be odd. The basic sequence of the k-stage Smolyak algorithm Q^{del} is regularly a.m. for degree $2k + 1$ if and only if $k \le 5$. It is the unique regularly a.m. basic sequence (of 6 formulae) if $k = 5$. For $k = 7$, the basic sequence of a regularly a.m. Smolyak algorithm consists of the first 6 formulae of the delay sequence. $Q^{(7)} = Q^{(8)}$ is an extension of Q_7^{KP} with 6 additional nodes and has negative coefficients. For larger k, the formulae $Q^{(1)}, \ldots, Q^{(8)}$ are as described before and $Q^{(9)}$ has to be a* 17*-point formula.*

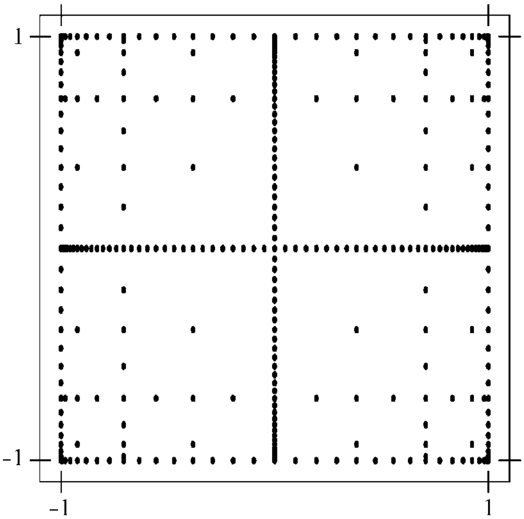

Fig. 1. The 321 nodes of $Q^{CC}(8, 2)$ (degree 15)

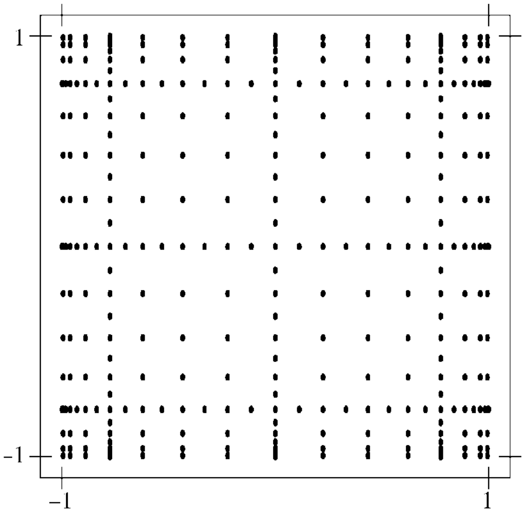

Fig. 2. The 321 nodes of $Q^{del}(16, 2)$ (degree 29)

Proof. Since k is odd, Theorem 2.1.) shows that we can apply Theorem 3b. Therefore, $Q^{(1)}[f] = f(1/2)$. From $\deg(Q^{(2)}) \geq 3$ it follows that $Q^{(2)}$ must have at least 2 additional nodes. For a regularly a.m. basic sequence of degree 3, we can take any symmetric 3-point formula of interpolatory type. However, the only 3-point quadrature formula of degree 5, i.e., the only 3-point quadrature formula that allows δ_2 to be zero, is the Gaussian. For the regular minimality of higher degree, we therefore have to choose $Q^{(2)} = Q^{(3)}$ and then to switch to a formula of higher degree. Since quadrature formulae of interpolatory type are uniquely determined by their nodes and the property $\deg(Q_n) \geq n-1$, all extensions of Q_3^G having at most 6 nodes and being of degree at least 5 are again Q_3^G. Therefore, $Q^{(4)}$ can be any extension of Q_3^G with 4 additional nodes and of interpolatory type. In order to generate further regularly a.m. formulae, we have to choose the 7-point quadrature formula with highest possible degree to make $\delta_4 = \delta_5 = 0$. This is the Kronrod extension of degree 11, i.e., $Q^{(4)} = Q^{(5)} = Q^{(6)} = Q_7^{KP}$. Of course, now, each extension of Q_7^{KP} with 6 additional nodes and of interpolatory type is a valid extension with fewer nodes than Q_{15}^{KP} and a further extension gives a sequence with asymptotically less nodes than Q^{del}.

In order to obtain a 13 point extension of Q_7^{KP} of degree 13+s, it is necessary and sufficient to find a monic polynomial $p \in \mathbb{P}_6$ satisfying

$$\int_{-1}^{1} E_4(x) P_3(x) p(x) x^\nu \, dx = 0, \qquad \nu = 0, \ldots, s \tag{47}$$

and having 6 zeros in $[-1,1]$ (see Brass [1, Theorem 55]). Here, P_3 is the Legendre polynomial of degree 3 and E_4 is the so-called Stieltjes-polynomial (see Monegato [7]), such that $E_4 P_3$ is the nodal polynomial of Q_7^{KP}. Then, the zeros of p are the additional nodes of $Q^{(7)}$. By explicit calculation, we obtain

$$E_4(x) P_3(x) = \text{const} \cdot (4455 T_7 + 693 T_5 + 1015 T_3 + 1005 T_1)\,, \tag{48}$$

where T_ν is the Chebyshev polynomial (of the first kind) of degree ν. It is linear algebra to show that all monic polynomials $x^6 + q(x)$, $q \in \mathbb{P}_5$, satisfying (31) with $s = 4$ have the form

$$\frac{1}{32}\Big(T_6(x) + \frac{24}{11} T_4(x) + \frac{58431}{10285} T_2(x) + c\Big) \tag{49}$$

with an arbitrary constant c. These functions are monotonically decreasing for $x < 0$, increasing for $x > 0$ and its second derivative at $x = 0$ is positive. Therefore, none of these functions has all its zeros in $[-1,1]$. On the other hand, requiring (47) with $s = 2$, we have

$$p(x) = \frac{1}{32}\Big(T_6(x) + \frac{24}{11} T_4(x) + a T_2(x) + b\Big). \tag{50}$$

p has 6 zeros in $[-1,1]$ if (a,b) is in a neighbourhood of $(3.5, 2)$. Therefore we have an extension with 6 additional nodes that is of degree 15. Any further regularly minimal extension of this sequence has to continue with $Q^{(8)} = Q^{(7)}$ and an extension of the 13-point formula, that is of degree 17. This must be a 17-point formula of interpolatory type.

We still have to show that each of the possible $Q^{(7)} = Q_{13}$ has a negative coefficient. By (50), the nodal polynomial of the additional nodes 6 nodes z_ν in Q_{13} is of the form

$$\begin{aligned} p(x) &= x^6 - \frac{9}{44}x^4 + cx^2 + d \\ &= (x^2 - z_1^2)(x^2 - z_2^2)(x^2 - z_3^2) \\ &= x^6 - (z_1^2 + z_2^2 + z_3^2)x^4 + \dots \end{aligned} \tag{51}$$

If it has 6 real zeros, then, $z_\nu^2 \leq 9/44$ or $z_\nu \leq \sqrt{9/44}$. Calculating also the nodes of Q_7^{KP} and of the Gaussian formula Q_8^G, we obtain that no node of Q_{13} is between the 7th node $x_{7,8}^G$ and the 8th node $x_{8,8}^G$ of the 8-point Gaussian formula. But, each positive quadrature formula of degree ≥ 15 must have at least one node in $[x_{7,8}^G x_{8,8}^G]$ (see Brass [1, Theorem 61]), which means that Q_{13} cannot be positive. □

Theorem 5 *The basic sequence of the k-stage Smolyak algorithm Q^{del} is regularly p-a.m. for degree $2k+1$ if and only if $k \leq 5$. For $k = 6$, we have $\delta_6 = 6$.*

Proof. By Theorem 3a, the proof is almost contained in that of Theorem 4. We only have to note that the quadrature formula of interpolatory type with the nodes of Q_7^{KP} plus the nodes $\pm 0.3,\ \pm 0.6$ and ± 0.85 is positive, which can be shown numerically. □

Corollary 4 *A regularly a.m. minimal basic sequence for degree $2k+1 \geq 15$ cannot be positive.*

Now, we want to show that the second case in Theorem 2.3c) may really occur.

Example 1 We construct a regularly a.m. sequence for degree 5 with $R^{(2)}[()^2] \neq 0$. If the Smolyak formulae are regularly a.m., they must have 2 stages. By Theorem 2, all basic formulae have to be exact for $\mathbb{P}_1$ and $Q^{(1)}[f] = f(1/2)$. We have

$$0 = R(3,1)[()^3] = R^{(3)}[()^3].$$

By Theorem 55 in Brass [1], the nodal polynomial $p(x) = (x - 1/2)(x - x_2)(x - x_3)$ must have mean value zero, such that $x_2 + x_3 = 1$. Since $Q^{(2)}$ also has to be based on the nodes $1/2,\ x_2,\ x_3$ and since $R^{(i)}[()^1] = 0$, all basic formulae must be symmetric. We only have to require that

$$Q^{(2)}[()^2] = 1/6 \qquad \text{and} \qquad \deg(Q^{(3)}) \geq 5. \tag{52}$$

The resulting sequence then gives a Smolyak algorithm of degree ≥ 5, if the latter is exact for $()^2 \otimes ()^2$. If we assume that $\delta_2 + \delta_3 \leq 3$ the problem is solved uniquely by $Q^{(3)} = Q_3^G$ and

$$(53) \qquad Q^{(2)}[f] = \frac{28}{18} f(\frac{1}{2}) - \frac{5}{18}\left[f(\frac{1}{2} + \sqrt{\frac{3}{20}}) + f(\frac{1}{2} - \sqrt{\frac{3}{20}}) \right].$$

A similar example exists for degree 9. In both examples, we obtain the same number of nodes as for Q^{del}. Numerical examples show only minor differences between Q^{del} and Smolyak quadrature (say $Q^{[5]}$ and $Q^{[9]}$) with the above nonpositive basic sequences For example, we have $\|Q^{del}(54, 50)\| \approx 9.5 \cdot 10^6$ and $\|Q^{[9]}(54, 50)\| \approx 4.4 \cdot 10^7$.

Corollary 5 *Q^{del} is regularly a.m. for all odd degrees less than 13.*

Hence, according to Theorem 3b, we know that the first 5 formulae of the basic sequence of Q^{del} are optimally chosen. Theorem 1 shows that the number of nodes induced by a regularly a.m. basic sequence for degree $2k + 1$ is a polynomial of degree k in d and the coefficients of the highest for monomials in this polynomial are the same as for Q^{del}. Therefore, there is only little space left for improvement, if we are looking for Smolyak formulae of given polynomial exactness involving as few nodes as possible. We summarize

Corollary 6 *Let $n^{min}(d + k, d)$ denote the numbers of nodes used by a formulae corresponding to regularly a.m. sequence. Then,*

$$\frac{n^{del}(d + k, d)}{n^{min}(d + k, d)} = 1 + O(d^{-5})$$

for fixed k.

Remark Finally, we mention that regular asymptotic minimality does not imply minimality in general.

1. In dimension one, for $k > 1$, Q_{k+1}^G uses fewer nodes than $Q^{del}(1+k, 1)$ to be exact for $\mathbb{P}_{2k+1}$.
2. Setting $Q^{(1)} = Q_2^G$, we have for the formulae $Q(2, 2)$ and $Q^{del}(3, 2)$ of degree 3 that $n(2, 2) = 4$ but $n^{del}(3, 2) = 5$ respectively.
3. Two Smolyak algorithms of degree ≥ 5 are the regularly a.m. $Q^{del}(d + 2, d)$ as well as $Q(d + 5, d)$ given by the basic sequence

$$Q^{(1)}[f] = f\left(\frac{1}{2} + \frac{1}{\sqrt{12}}\right)$$
$$Q^{(2)}[f] = Q_2^G[f] = \frac{1}{2}\Big[f\left(\frac{1}{2} - \frac{1}{\sqrt{12}}\right) + f\left(\frac{1}{2} + \frac{1}{\sqrt{12}}\right) \Big]$$
$$Q^{(3)} = Q^{(4)} = Q^{(5)} = Q^{(2)}$$

and

$$Q^{(6)} = Q_5^{KP}.$$

We have $n(d+5,d) < n^{del}(d+2,d)$ for $d = 3,4,5$.

5 Numerical examples in the unweighted case

As examples, we consider integration over the d-dimensional unit cube for different basic sequences. In Fig. 3 we compare the right-hand side coefficients $\varepsilon(d+k,d,r)$ of error bounds in (7) given by the procedure in [13].

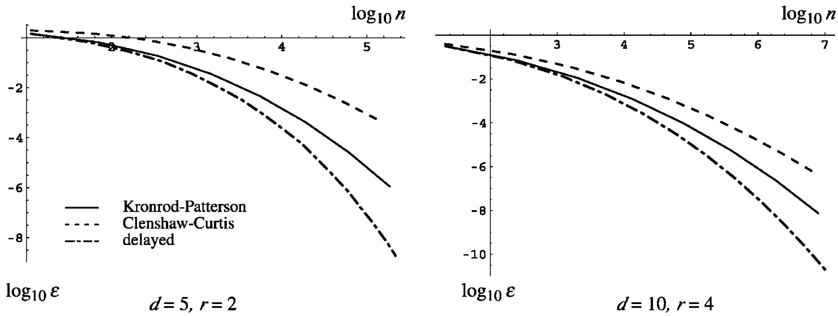

Fig. 3. Error bounds; $n := n(d+k,d)$ and $\varepsilon = \varepsilon(d+k,d,r)$

Now, we take the smooth examples from a frequently used test package that has also been used, e.g., by Sloan and Joe [14] and by Novak and Ritter [9]. In each of the examples, we made 21 tests with parameters randomly chosen. The respective numbers of correct digits are

$$(58) \qquad \mathrm{dig}_n[f] := -\log_{10}\left|\frac{R(d+k,d)[f]}{I_d[f]}\right|, \qquad n = n(d+k,d).$$

and we denote by dig_n the respective medians of $\mathrm{dig}_n[f]$ for the 21 tests. The functions are in the following families

OSCILLATORY $\quad f_1(t) = \cos\left(2\pi w_1 + \sum_{i=1}^{d} c_i t_i\right), \quad \sum c_i = 9$

PRODUCT PEAK $\quad f_2(t) = \prod_{i=1}^{d} \frac{1}{c_i^{-2} + (t_i - w_i)^2}, \quad \sum c_i = 7.25$

CORNER PEAK $\quad f_3(x) = \left(1 + \sum_{i=1}^{d} c_i t_i\right)^{-d-1}, \quad \sum c_i = 1.85$

GAUSSIAN $\quad f_4(t) = \exp\left(-\sum_{i=1}^{d} c_i^2 (t_i - w_i)^2\right), \quad \sum c_i = 7.03$

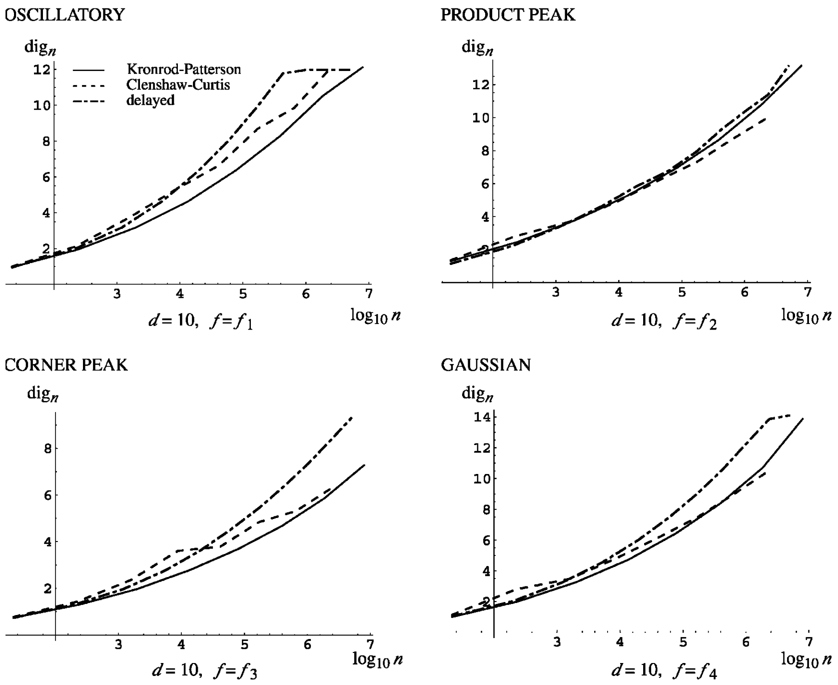

Fig. 4. Correct digits for sample functions; $n := n(d + k, d)$

Some samples from the tests are shown on Fig. 4.
Note that in these examples, the delay algorithm needs between 3.3 and 8 times less nodes than $Q^{KP}(18, 10)$ and $Q^{CC}(19, 10)$ to reach the same median of precision, except for the product peak function and the comparison with Q^{KP}, where the delay algorithm shows approximately the same error behaviour as Q^{KP}. Corresponding examples for non-smooth test functions show a superiority of the non-delayed Smolyak basic sequences. This indicates that the delayed algorithm uses too few function values along the main axes. We recommend in such either non-delayed sequences or sequence of numbers of nodes with only little delay, e.g., $1, 3, 3, 7, 15, \ldots$ or $1, 3, 3, 7, 7, 15, 31, \ldots$. The numbers of nodes of the Smolyak algorithm are then reduced compared with the non-delayed formulae, while the convergence in univariate directions seems to be faster than for the delayed algorithm. We compare the calculations with the above-used formulas with those with the Smolyak formulas based on Kronrod-Patterson formulas using $1, 3, 3, 7, 15, 31, 31, 63, 63, 63, 63$ nodes respectively. It appears that these Smolyak algorithms with only little delay are more competitive than the delay algorithms.

For Fig. 5 we used the families

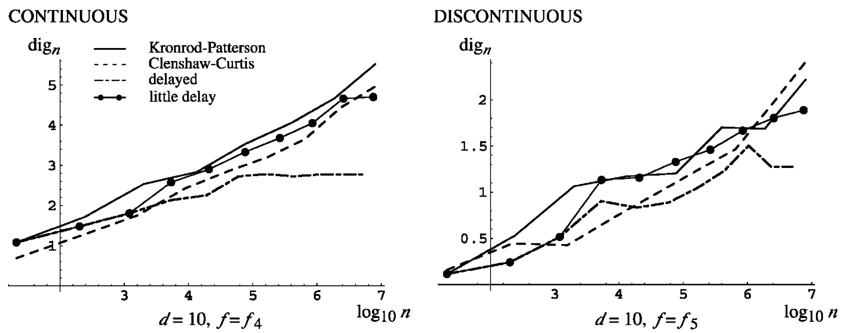

Fig. 5. Correct digits for non-smooth sample functions; $n := n(d+k, d)$

CONTINUOUS

$$f_5(t) = \exp\left(-\sum_{i=1}^{d} c_i |t_i - w_i|\right), \qquad \sum c_i = 20.4$$

DISCONTINUOUS

$$f_6(t) = \begin{cases} 0 & \text{if } t_1 > w_1 \text{ or } t_2 > w_2 \\ \exp\left(\sum_{i=1}^{d} c_i x_i\right) & \text{otherwise} \end{cases}, \qquad \sum c_i = 4.3$$

Remark Let us mention, that in [13, Example 1], we have proved, e.g., that for a sample from the family GAUSSIAN, we obtain the error bound

$$|R^{KP}(18, 10)[f]| \leq 5.3 \cdot 10^{-7} \tag{59}$$

(and a relative error bound $\leq 2.2 \cdot 10^{-6}$), where we have used $n = 8\,085\,505$ function evaluations. Analogously, one can show that

$$|R^{del}(21, 10)[f]| \leq 4.6 \cdot 10^{-9} \tag{60}$$

(relative error bound $\leq 2 \cdot 10^{-8}$) with $n = 5\,020\,449$ function evaluations.

In Fig. 6 we illustrate that asymptotically minimal algorithms not necessarily show their superiority for high dimensions. The reason is that $n(d+k, d)$ of all Smolyak algorithms with $\delta_0 = 1$ and $\delta_1 = 2$ has the same main coefficient as a polynomial of d. In particular, the effort for Clenshaw-Curtis- and Gauss-Kronrod-based Smolyak algorithms in high dimensions is not much bigger than that for the delay Smolyak algorithm. The results in dimension 10 for the ocillatory integrand have already been listed. Now, we do the same for dimensions 6 and 18.

The "classical" Gauss-Kronrod-based Smolyak method seems to lose its effectiveness in higher dimensions due to the fast increasing number

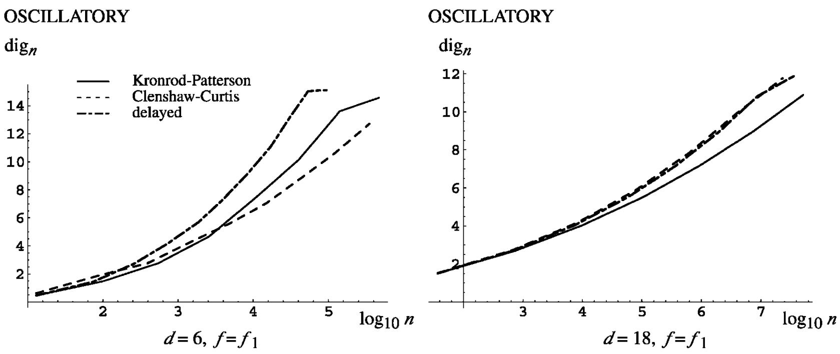

Fig. 6. Correct digits for sample functions; $n := n(d+k, d)$

of nodes. In all smooth examples for dimesion 18, there were only minor differences between the results for Clenshaw-Curtis and for the delayed sequence.

6 An example from finance

Often, financial applications have a very high dimension. There is some evidence (see Sloan and Woźniakowski [15]) that these problems are only tractable, if some dimensions are less important than others. In that case, it is useful to use a smaller number of nodes in less important directions. This approach has been considered, e.g., in Wasilkowski and Woźniakowski [18] or [19] and Novak, Ritter and Steinbauer [11]. We may try to learn from the results above and repeat quadrature formulae in the basic sequence. Since the upper dimensions in the example are less important, we repeat the quadrature more often for these dimensions in order to save function evaluations. Again, we choose basic formulae among Kronrod-Patterson formulae. Table 2 shows, how often a certain Kronrod-Patterson formula is in the basic sequence for the respective dimensions in our example.

The respective numbers of nodes of $Q(360+k, 360)$, $k = 1, \ldots, 7$ are 11, 71, 413, 2241, 11433, 54757, 247017.

Table 2. Occurences in the basic sequence

dimension	Q_1^{KP}	Q_3^{KP}	Q_7^{KP}	Q_{15}^{KP}	Q_{31}^{KP}
1	1	1	2	3	4
2..5	1	2	3	4	5
6..13	2	3	4	5	6
14..40	3	4	5	6	7
41..120	4	5	6	7	8
121..360	5	6	7	8	9

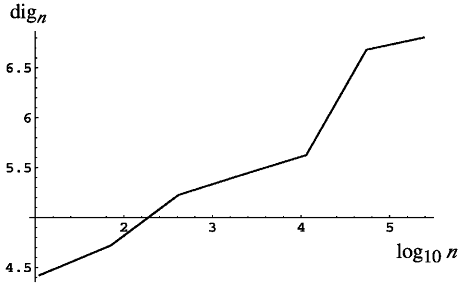

Fig. 7. Correct digits dig_n for MBS-integral; $n := n(d+k, d)$

The arguments in Sect. 3 concerning the polynomial degree are therefore no longer relevant. Nevertheless, we might hope to learn from the unweighted case. As an example, we consider an example for valuing Mortgage-Backed-Securities (MBS, see Tezuka [17]).

We have the following curve for the numbers of correct digits (see Fig. 7). We see that already 413 function evaluations are sufficient to obtain a relative error less than $10^{-5.2}$ and with 54757 nodes, the relative error is less than $10^{-6.6}$. The Quasi-Monte-Carlo used by Tezuka [17] shows a slightly slower convergence. Near $n = 5000$ function evaluations, the relative errors are in a range from zero to about 10^{-5}. Both, Smolyak and Quasi-Monte-Carlo beat the Monte-Carlo method in this application.

7 Remarks on degenerate basic sequences

Most of the results in Sect. 3 have been obtained under the assumption that the basic sequence is regular. We now want to discuss briefly some changes in the case of m-degenerate basic sequences, i.e. of basic sequences with $\delta_1 = \ldots = \delta_m = 0 \neq \delta_{m+1}$.

1. The regular k-stage formulae can be considered as a subclass of m-degenerate formulae. Namely if we have a regular basic sequence $Q^{(1)}$, ..., we can define $\widetilde{Q}^{(\mu(m+1)+\nu)} := Q^{(\mu+1)}$ for $\mu = 0, 1, \ldots$ and $\nu = 1, 2, \ldots, m+1$. The corresponding $k(m+1)$-stage m-degenerate algorithm is the same as the original k-stage algorithm.
2. The formulae (15) and (16) show that

$$\begin{aligned} c_{j,k} &= \frac{\delta_{m+1}}{\delta_0} c_{j-1,k-m-1} + \sum_{\nu=m+2}^{k-j+1} \frac{\delta_\nu}{\delta_0} c_{j-1,k-\nu} \\ &= \left(\frac{\delta_{m+1}}{\delta_0}\right)^2 c_{j-2,k-2(m+1)} \end{aligned}$$

$$+\sum_{\nu=m+2}^{k-j+1}\sum_{\mu=m+2}^{k-\nu-j+2}\frac{\delta_\mu\delta_\nu}{\delta_0^2}c_{j-2,k-\nu-\mu}$$

$$= \dots \tag{61}$$

does not vanish only if $k \geq j(m+1)$. This means that the m-degenerate Smolyak formula $Q(d+s(m+1),d)$ has approximately as many nodes as the regular Smolyak formula $\widetilde{Q}(d+s,d)$ if $\delta_0 = \widetilde{\delta}_0$ and $\delta_{m+1} = \widetilde{\delta}_1$. Hence, we have much less nodes for a given number of stages. On the other hand, we need $m+1$ times as many stages in order to obtain the same degree:

3. In the same way as for regular formulae, we can prove that, with a m-degenerate basic sequence, a degree of exactness $\geq 2k+1$ can only be achieved for infinitely many dimensions, if
   (i) $Q^{(1)}$ is exact for linear functions
   (ii) The Smolyak formula has at least $k(m+1)$ stages
   (iii) The determining equation for $Q^{(m+1)}[()^2]$ of a m-degenerate $k(m+1)$-stage Smolyak algorithm of degree $\geq 2k+1$ is the same as for $Q^{(2)}[()^2]$ of a regular k-stage Smolyak algorithm. Hence $\delta_{m+1} \geq 2$. Therefore, for the number of nodes for those formulae is determined by a polynomial of degree k with main coefficient $(\delta_{m+1}/\delta_0)^k$, i.e., with the same main coefficient as regularly a.m. basic sequences.
   (iv) Suppose we have a (1-degenerate) basic sequence with $\delta_0 = 1$, $\delta_1 = 0$, $0 < \delta_2 \leq 2$, $\sum_{\nu=0}^{5}\delta_\nu \leq 3$ and $\sum_{\nu=0}^{6}\delta_\nu \leq 7$. We can solve the equations that are necessary for the corresponding Smolyak formula to be of degree ≥ 7 with, e.g., MATHEMATICA, and obtain that $\delta_2 = 2$ and that $Q^{(3)}$ uses the nodes of Q_3^G. Since $Q^{(7)}$ has to be of degree ≥ 7, we can argue as in the regular case that $\delta_6 = 4$. Therefore, we know that any 1-degenerate algorithm with $\deg(Q(d+k,d)) \geq 7$ for all d uses asymptotically as least as many nodes as a regular a.m. algorithm for degree 7.

At this point, we can not decide, whether there are (degenerate) a.m. basic sequences yielding the same degree of exactness but use less nodes than regularly a.m. basic sequences. This might be topic of further investigations.

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