STRONGLY NESTED 1D INTERPOLATORY QUADRATURE AND EXTENSION TO ND VIA SMOLYAK METHOD

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Key words: Integration, nested quadrature rules, Smolyak sparse grids

Abstract. One dimensional interpolatory rules with n to n+2 nesting are first derived by local and global minimization of the classical bounds of integration and polynomial interpolation error. The proposed 1D rules are then tested for different classes of functions. The most efficient 1D quadratures are then extended to multi-dimension using Smolyak's method and tested on basic multivariate functions. The proposed rules and their nD extension appear to be as efficient as their counterparts based on the classical Leja sequences. A more complete presentation of this work is available in [5]

1 INTRODUCTION

A very large number of scientific problems require the calculation of integrals and this need has led to the development and analysis of various types of quadrature formulae [3]. In the framework of interpolatory quadrature rules, the so-called nested formulae are those in which the points of a coarse set are included in larger sets defining more accurate formulae. This property is highly desirable when the evaluation of the function of interest is expensive, e.q. when it is an output of a CPU-expensive numerical simulation.

The most often used 1D nested quadratures are two interpolatory rules : Fejér second rule [8] for which the nesting property is obtained from *n*-point set to (2n+1)- point set, and Clenshaw-Curtis rule [1] that has a *n* to (2n - 1) nesting. The aim of this work is to propose and study symmetric interpolatory quadratures with a *n* to n + 2 nesting property. They are also compared with interpolatory rules based on Leja-sequences that are the reference for strongly nested rules.

In section 2, basics about interpolatory quadrature and Gauss-Legendre quadrature are recalled. In section 3, notions about all classical nested quadratures are introduced. In section 4, the mathematical criteria that have appeared in section 2 and 3 in mathematical

analysis of interpolatory quadratures are used to derive n to n+2 nested sets of 33 points by successive or global minimization. The proposed 1D rules are tested and compared with classical rules in section 5. Section 6 recalls the main properties of Smolyak sparse grids illustrating this complex technique with detailed 2D examples. Finally in section 7, the best 1D quadratures are extended in multi-dimension with Smolyak's method and tested on basic multivariate functions.

2 Interpolatory quadrature and Gauss-Legendre quadrature

2.1 Interpolatory quadrature rules

By a linear change of variable a finite summation interval can be transformed to [-1, 1] so that, without restrictions, integrals like

$$S[f] = \int_{-1}^{1} f(x)dx$$

can be considered. An interpolatory rule [3, 2] is of the form

$$S[f] \simeq I_n[f] = \sum_{i=1}^n w_i f(x_i) \tag{1}$$

where $x_1 < x_2 < ... < x_n$ are distinct nodes (their set being denoted S_n) and $w_1, w_2...w_n$ are the corresponding weights. The weights are defined so that all monomials of the canonic polynomial basis $1, x, x^2...x^{n-1}$ are exactly integrated. They appear as the solution of the corresponding linear system and also as the integrals of Lagrange polynomials

$$L_n^i(x) = \prod_{l=1; l \neq i}^{l=n} \frac{(x - x_l)}{(x_i - x_l)} \qquad w_i = \int_{-1}^1 L_n^i(x) dx$$

It is easily checked that $I_n[f]$ is the exact integral of the polynomial that interpolates f at the nodes which establishes a link between accuracy of polynomial interpolation and accuracy of interpolatory rules.

2.2 Accuracy of interpolatory rules

The error in the evaluation of the sum S[f] by $I_n[f]$ is now denoted $R_n[f]$

$$R_n[f] = \int_{-1}^{1} f(u) du - \sum_{i=1}^{n} w_i f(x_i)$$

The classical bounds of $R_n[f]$ for a C^0 , C^r and C^r (r < n) function are recalled and discussed in [5]

2.3 Minimal Lebesgue constant and derived criteria for interpolation and integration accuracy

It is known that not all sets of points are well suited for interpolation and interpolatory quadrature: uniformly-distributed points, for example, is known to be a bad choice, for which large interpolation error may appear at boundaries for regular functions and large integration errors are observed [3]. The purpose of this section is to present criteria to derive sets of points that do not suffer from these issues. The Lebesgue constant Λ_n of a sequence of n distinct points gives an indication on the quality of polynomial interpolation based on this set. Let us denote b_{n-1} the best polynomial approximation of degree n-1for a fixed norm of the continuous function f. More, precisely, the Lebesgue constant, denoted here Λ_n , is bounding the interpolation error following

$$||f - \Pi_n(f)|| \le (\Lambda_n + 1)||f - b_{n-1}||$$
(2)

The advantage of using a sequence of points exhibiting low Lebesgue constant for interpolation is then obvious. An explicit expression of Λ_n is most often derived for the infinity norm, for which last equation yields

$$\Lambda_n = \max_{x \in [-1,1]} Leb^n(x) \qquad Leb^n(x) = \sum_{j=1}^n |L^j(x)|$$
(3)

and

$$||f - \Pi_n(f)||_{\infty} \le (1 + \Lambda_n) E_{n-1} \quad |R_n[f]| \le (2 + 2\Lambda_n) E_{n-1}.$$
(4)

where $E_{n-1} = ||f - b_{n-1}||_{\infty}$. In case the Lebesgue function of the set $Leb^n(x)$, has a localy a very high value (see [5] figure 1) the bound of $|R_n[f]|$ in equation (4) may be very pessimistic and less satisfactory than another easily derived bound for $|R_n[f]|$,

$$|R_n[f]| \le \left(2 + \int_{-1}^1 Leb^n(x)dx\right) E_{n-1}$$
(5)

2.4 Gauss-Legendre quadrature

As discussed in previous section, interpolatory rules based on sets of n points exactly integrate polynomials of degree n - 1. Besides, n-point Gauss-Legendre rule exactly integrate polynomials of degree up to 2n - 1. The actual superiority of Gauss Legendre quadrature for non polynomial functions has been discussed by Trefethen [14]. Definition and extensive properties of Gauss Legendre rule can be found in [3]. Definition and main properpies are recalled in [5]

3 Nested quadrature rules

In some cases, a very reliable value of S[f] is needed so that formulae of increasing accuracy should be used up to obtaining a sufficiently converged evaluation. If the calculation of $f(x_i)$ is expensive, it is highly desirable that all (or at least some) of the nodes of the *n*-point rule are also involved in some of the further (n + p)-point rules. If so, the rules and sets of nodes are said to be nested.

This property is rather rare. The basic version of Gauss-Legendre quadrature do not have this property but nested extensions (more nodes) or restrictions (less nodes) exist and are presented in [5] §3.3.

The two classical nested interpolatory rules are the second rule of Fejér [8] and the rule of Clenshaw and Curtis [1] that respectively satisfy $S_n \subset S_{2n+1}$ and $S_n \subset S_{2n-1}$. The nodes of the *n*-point second rule of Fejér are the roots of the second-kind Chebychev polynomial $U_n(x)$. The *n*-point rule of Clenshaw and Curtis has the same abscissae as the (n-2)-rule of Fejér plus the two extrema -1 and +1. The precise definition of these two rules can be found in [3] or [2].

Besides, sequences of points with a stronger nesting property $-S_n \subset S_{n+1}$ or $S_n \subset S_{n+2}$ – may be used for polynomial interpolation. The classical option is Leja sequence. Its definition in an interval T of \mathbb{R} reads

$$x_{n+1} = \arg \max_{x \in T} \left| \prod_{i=1}^{n} (x - x_i) \right|$$
(6)

where the first point, x_0 , is chosen arbitrarily in T. Even when started by 0 in a symmetric interval, this recursive process does not successively add opposite points to the set.¹

In order to compare Leja-based interpolatory quadrature to symmetric quatradures, it may be convenient to define a symmetric Leja-type set of points. In the interval [-1,1], the straighforward definition of this sequence is

$$x_{n+1} = \underset{x_{n+1} \ x_{n+2} = -x_{n+1}}{\operatorname{Arg max}} \left| (x_{n+2} - x_{n+1}) \prod_{1 \le j \le n} (x_{n+1} - x_j) \prod_{1 \le i \le n} (x_{n+2} - x_i) \right|$$
(7)

Actually many options and variants exist. The symmetric and non-symmetric Leja sequences used for the tests are explicitly defined in §4.3.

4 Definition of n/n+2 nested sets of points for interpolatory quadrature from global criteria

In an earlier work [4], Dumont built symmetric sequences of points starting from $\{-1, 0, 1\}$ by successive minimization of different critera (Lebesgue constant, integral of Lebesgue function, integral of absolute value of nodal polynomial, infinity norm of sum of squared Lagrange polynomials...). He then assessed the efficiency of the corresponding interpolatory rules for the six test function of a classical article by Trefethen [14]. This first set of results validates the decision to focus for further study on:

- succesive and global minimization of Lebesgue constant;

- successive and global minimization of integral of Lebesgue function;

¹As an example, starting with $x_1 = 0$ yields $x_2 = 1$ (or -1 resulting of the maximization of |x|), then $x_3 = -1$ (resulting of the maximization of |(x - 1)x|), then $x_4 = \frac{1}{\sqrt{3}} = 0.577350$. (resulting of the maximization of |(x - 1)(x + 1)x|; its opposite $-1/\sqrt{3}$ may have been chosen); then $x_5 = -0.658706$. is found by maximization of $|(x - 1)(x + 1)(x + 1)(x - \frac{1}{\sqrt{3}})x|$. None of the next points, considered two by two, are opposite one of each other

– Leja sequences where the the argmin of infinity norm of nodal polynomial is successively add to current set.

4.1 Successive and global minimization of Lebesgue constant

The symmetric sequence starting with $S_3 = \{0, -1, 1\}$ and minimizing successively the Lebesgue constant has been derived up to n = 257. The first 33 values are printed hereafter

```
\begin{split} \mathcal{S}^{LebConst-so}_{33} = \{ & 0, -1, 1, \\ & \pm \ 0.620911304689912, \pm \ 0.851116906275467, \pm \ 0.366893560557081, \pm \ 0.949647785059444, \\ & \pm \ 0.228417726292775, \pm \ 0.726262806499719, \pm \ 0.982331094378673, \pm \ 0.476576613596911, \\ & \pm \ 0.796922940675856, \pm \ 0.131045085133918, \pm \ 0.913065535238725, \pm \ 0.555583265445366, \\ & \pm \ 0.994175387122204, \pm \ 0.303955266207398, \pm \ 0.683362049812905 \} \end{split}
```

The Lebesgue constants, integrals of Lebesgue function and infinity norm of nodal polynomials are plotted in figure 4.1 for corresponding nested sequences with cardinal 1 to 257. On all of the figures, the quantity of interest is also plotted for Clenshaw-Curtis quadrature (although its nesting is (n to 2n - 1) and hence different and lower from the one studied). On the last plot, the optimal infinity norm obtained with first-kind Chebyshev polynomial is also plotted.

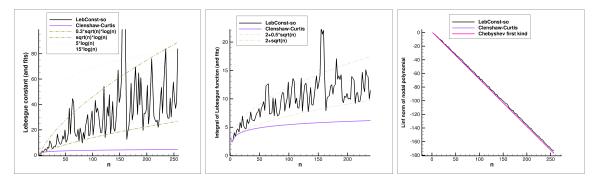


Figure 1: Lebesgue constant, integral of Lebesgue function and Linf norm of nodal polynomial for LebConst - so sequence of sets

It is first to be noted that the infinity norm of nodal functions is very weakly discriminant : it is almost the same for the three considered sequences of points.

As concerning the integral of Lebesgue function Leb^n , as a function of cardinal n, it is much less regular for the proposed (n/n+2) nested sequence than for the Clenshaw-Curtis sets of points. The values of the sum are roughtly two times higher than those obtained for Clenshaw-Curtis sets of points.

Finally, the Lebesgue constant is the most discriminant quantity : Clenshaw-Curtis sets of points have a Lebesgue constant close the optimal one $(\Lambda_n \simeq 2/\Pi \log (n) + .7219 \simeq 0.6366 \log (n) + 0.7219)$ whereas the Lebesgue constant of the LebConst-so sets seems to be bounded by $\sqrt{(n)log(n)}$ curves.

Considering the strong irregularities of the Lebesgue constant on former left-plot it is decided to carry a global search for a 33-point set satisfying

$$\forall \ odd \ n \quad \Lambda_n \le 3 + K(\sqrt{n} \ \log(n) - \sqrt{2} \ \log 2) \tag{8}$$

the selected set being the one exhibiting the smallest K value. Please note that $\Lambda_3(\{-1, 0, 1\}) = 1.25$ and $\Lambda_2(\{0, 1\}) = 3$ which explains the form of the selected right-hand-side that aims at avoiding to be too restrictive on the first values of the set. The lowest K value that could be achieved is 0.2508. The corresponding sequence of points is given below

```
\begin{split} \mathcal{S}^{LebConst-go}_{33} = \{ & 0, -1, 1, \\ & \pm \ 0.782948160530396, \pm \ 0.442592038865533, \pm \ 0.952401768588314, \pm \ 0.289462405510965, \\ & \pm \ 0.631474499429657, \pm \ 0.900375626425636, \pm \ 0.139818101722143, \pm \ 0.984577322855455, \\ & \pm \ 0.723776947906398, \pm \ 0.524915574329834, \pm \ 0.860067776493385, \pm \ 0.204617156721863, \\ & \pm \ 0.997188614738299, \pm \ 0.376693743737914, \pm \ 0.817795412857899 \} \end{split}
```

This sequence of points is denoted hereafter *LebConst-go* where *go* stands for global optimization.

4.2 Successive and global minimization of Lebesgue function integral

The symmetric sequence starting with $S_3 = \{0, -1, 1\}$ and minimizing successively the integral of Lebesgue function Leb^n has been derived up to n = 257. The first 33 values of the sequence are written down hereafter

$$\begin{split} \mathcal{S}^{LebInt-so}_{33} = \{0,-1,1, & \pm \ 0.625636256324887, \pm \ 0.851846657718325, \pm \ 0.339641788238558, \pm \ 0.946850997383622, \\ & \pm \ 0.482106487818637, \pm \ 0.757667608694366, \pm \ 0.175376580400003, \pm \ 0.981012153711729, \\ & \pm \ 0.693525212879786, \pm \ 0.259992979486419, \pm \ 0.906365106082807, \pm \ 0.547932944191913, \\ & \pm \ 0.993631434395368, \pm \ 0.094661345500811, \pm \ 0.813221010757367\} \end{split}$$

The Lebesgue constants, integrals of Lebesgue function and infinity norm of nodal polynomials are plotted in figure 4.2 for corresponding nested sequences with cardinal 1 to n for all odd n up to 257. On all of the figures, the quantity of interest is also plotted for Clenshaw-Curtis quadrature (although its nesting is (n to 2n - 1) and hence different and lower from the one studied). On the last plot, the (optimal) infinity norm obtained with first-kind Chebyshev polynomials is also plotted.

As in the previous subsection, it can first be noted that the infinity norm of nodal functions is very weakly discriminant : it is almost the same for the three considered sequences of points (and from previous subsection, LebInt - so and LebConst - so sequences also exhibit very close Linf norm values).

As concerning the integral of Lebesgue function Leb^n , that has been successively minimized for this sequence of points, the values for LebInt - so are not that different from those obtained with LebConst - so and are also much less regular than for Clenshaw-Curtis sets of points. Once again the values of the sum are roughly two times higher than those obtained for Clenshaw-Curtis sets of points.

Finally, the Lebesgue constant of the LebInt - so sequence are extremely high for n larger-equal 41 (see left plot, all values are then larger than 1000.) It is understandable

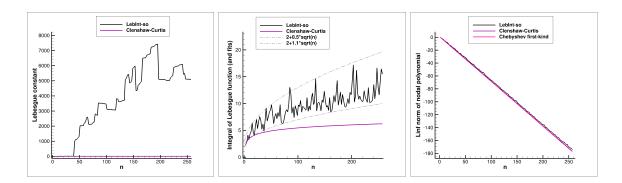


Figure 2: Lebesgue constant, integral of Lebesgue function and Linf norm of nodal polynomial for LebInt - so sequence of sets

that bounding the sum of Lebesgue function does not imply small maxima (these maxima being potentially reached inside a narrow interval of two successive points).

Considering the strong irregularities of Lebesgue function integrals on former middleplot it is decided to carry a global search for a symmetric 33-point set satisfying

$$\forall \ odd \ n \qquad \int_{-1}^{1} Leb^n(u) du \le 2.5 + M\sqrt{n} \tag{9}$$

the selected set being the one exhibiting the smallest M value. Please note that integral of Lebesgue function for $S_3 = \{0, -1, 1\}$ is 7./3. so that the 2.5 factor slightly relesases the casting of the first values. The lowest M value that could be achieved is 0.6345. The corresponding sequence of points is given below

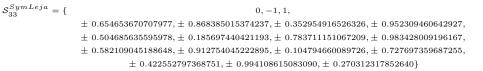
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\begin{split} \mathcal{S}^{LebInt-go}_{33} = \{ & 0, -1, 1, \\ & \pm 0.742273664520371, \pm 0.444637291229912, \pm 0.937057846443702, \pm 0.200751204315954, \\ & \pm 0.826628128579930, \pm 0.564901505415219, \pm 0.983338034692550, \pm 0.303389608312067, \\ & \pm 0.899144224779301, \pm 0.666061882265197, \pm 0.108065516925028, \pm 0.972940266528069, \\ & \pm 0.517131356717868, \pm 0.856338439158728, \pm 0.359707318113626 \} \end{split}
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This sequence of points is denoted herefater *LebInt-go* where *go* stands for global optimization.

4.3 Successive minimization of Linf norm of nodal polynomial (Leja sequence)

The Lebesgue constants, integrals of Lebesgue function and infinity norm of nodal polynomials are plotted for Leja sets – equation (6) starting from $\{-1, 0, 1, 1/\sqrt{3}\}$ – and symmetric-Leja sets – equation (7) starting from $\{-1, 0, 1\}$. The considered values of the cardinal are odd values up to 513 for symmetric-Leja and all odd or even values up to 513 for standard Leja. The first thirty-three abscissae of the two sequences are given hereafter. In the plots of next section, Leja and symLeja will refer to these two sequences of points.

 $S^{Leja}_{33} = \{0, -1, 1, 0.577350263138291, -0.658706600365785, 0.839254171100097, -0.870007151554750, -0.305613333872171, 0.32170760667263, 0.942979180631893, -0.952673271979931, -0.479412332060666, 0.712638635138148, 0.155959361490346, -0.774872345699519, 0.979477618088481, -0.161165271379463, -0.983326309910829, 0.461370596797464, 0.891892818173957, -0.571897089258940, -0.912559745086007, 0.649253519653005, -0.079817976235472, 0.242306534869635, -0.722294392331989, 0.992668623512365, -0.390789519100806, 0.782130683608553, -0.994056747611527, 0.397576889604314, -0.826384680543965, 0.920048378946020\}$



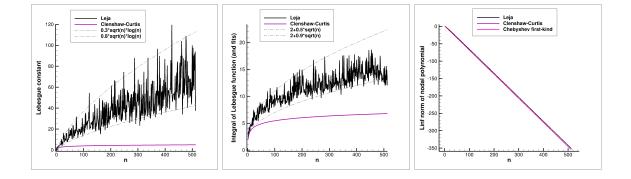


Figure 3: Lebesgue constant, integral of Lebesgue function and Linf norm of nodal polynomial for Leja sequence of sets

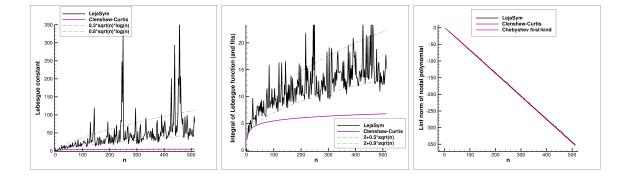


Figure 4: Lebesgue constant, integral of Lebesgue function and Linf norm of nodal polynomial for symmetric Leja sequence of sets

Considering figures 3 and 4, it can first be noted, once again, that the infinity norm of nodal polynomials is very weakly discriminant : its values are almost the same for Leja and symLeja as for $LebInt - so \ LebConst - so$ and are also very close to those of Chebyshev first-kind polynomial and Clenshaw-Curtis sets of nodes.

Looking at Lebesgue constant values, it is observed that symmetric-Leja sequence exhibits isolated very high values (way larger than the $0.8\sqrt{n}\log(n)$ curve proposed for reference) that do not appear for non-symmetric Leja. Surprisingly, Lebesgue constants are (in average over some neighbours of each point) smaller for Leja sequence than for LebConst-so (see position w.r.t. upper reference curves and definition of these curves).

As considering integral of Lebesgue function, the two plots have been seconded by $2+K\sqrt{n}$ reference curves although for the Leja sequence, a lower exponent may have been more appropriate (see central plot in figure 3). It is observed that the symmetric Leja sequence exhibits significantly higher values of integral of Lebesgue function than LebInt - so sequence whereas those of the classical non-symmetric sequence have the same order of magnitude as those of LebInt - so.

5 Test for classical 1D functions

Convergence of integration rules towards the exact sum value (when increasing the number of quadrature points) strongly depends on the regularity of the function. Quadrature rules should hence be tested for different types of functions : (a) polynomials, which allow to check the properties of polynomial exactness ; (b) entire functions, in our tests, exponentials, exponential of a polynom, cos and linear combination of these ² ; (c) analytic and C^{∞} but not analytic functions ; (d) C^0 , C^1 and C^2 functions.

The proposed 1D n/n+2 nested interpolatory quadratures appeared to be as efficient as those based on Leja sequences for all types of functions. All these strongly nested quadrature are not as efficient as Gauss-Legendre, Clenshaw-Curtis and Fejer second rule for the integration of very regular functions.

The reader is referred to reference [5] §5 for a comprehensive presentation.

6 Extension to multi-dimension via Smolyak's method

The sections above discussed the definition and efficiency of four 1D interpolatory rules with respect to classical rules. Integration of functions of \mathbb{R}^d is now considered. The domain is supposed to be $[-1,1]^d$ and

$$Sum_{d}[f] = \int_{[-1,1]^{d}} f(x_{1},...,x_{d}) dx_{1}...dx_{d}$$

is to be numerically estimated for a continuous f. Only Smolyak's sparse grid method [13] based on the studied 1D interpolatory rules is considered. The reader is referred to [5] §5 for a detailed presentation of Smolyak's sparse grids.

7 Test of nD Smolyak quadratures for Genz functions

The coding of Smolyak sparse grids is quite technical and we rather rely on a package designed by Dwight et al. [6] which follows the indexing proposed in [11] and proposes tests for Genz functions [9]. Actually the domain of integration with this tool is $[0, 1]^d$ but

 $^{^{2}}$ although the type of these functions refers to complex analysis, these functions are considered here for real inputs

the simple conversion of 1d rule from [-1, 1] to [0, 1] is easily coded in this framework. Here, we retain the oscillatory function, F_1 , the "product peak" function, F_2 , the Gaussian function, F_4 , and the C^0 function F_5 ,

$$F_1 = \cos\left(2\Pi u_1 + \sum_{i=1}^{i=d} a_d x_i\right) \qquad F_2 = \frac{1}{\prod_{i=1}^{i=d} (1/a_d^2 + (x_i - u_i)^2)}$$

$$F_4 = \exp\left(-\sum_{i=1}^{i=a} a_d (x_i - u_i)^2\right) \qquad F_5 = \exp\left(-\sum_{i=1}^{i=a} a_d |x_i - 0.5|\right).$$

The *a* parameters are chosen equal for all coordinates but dependant on the dimension: a_d is equal to 4.5 for dimension 2, 1.8 for dimension 5 and 0.9 for dimension 10). The u_i are all taken equal to 0.5.

New Python classes, corresponding to LebConst-so, LebConst-go, LebInt-so, LebInt-go, Leja and symLeja 1D interpolatory rules are added to the "smobol" package [6] that then automatically builds sparse grids based on these 1D rules.

Tests are then carried out for the sparse grid rules based on LebConst-so, LebConst-go...symLeja rules (17 levels, from 1 to 33 points) and also Gauss-Patterson rule (6 levels respectively involving 1, 3, 7, 15, 31 and 63 points) and Clenshaw-Curtis rule (10 levels involing 1,3,5,9...513 points). Integral evaluations are requested to last less than a few minutes which actually limits the number of nodes per calculation to roughly one milion ; this is the reason why the highest level sparse grids are not tested in dimension 10. The results are gathered in figure 5 and 6.

For the analytic function F_1 and F^4 , and the C^{∞} function F^2 the convergence is faster for the sparse grid rules based on strongly nested quadratures (LebConst-so, LebConst-go, LebInt-so, LebInt-go, Leja symLeja) than for the one based on Clenshaw-Curtis but the difference is less significant in dimension 10 than in dimension 2 and 5 (see figure 5). For the C^0 function F^5 , the sparse grid rules based on strongly nested quadratures gives decreasing but weavy evaluation of the integral when increasing the level l. The Clenshaw-Curtis based sparse grid is in this case more efficient than those derived from the strongly nested quadrature (see figure 6).

8 Conclusion

One dimensionnal interpolatory quadratures have been proposed based on classical bounds on integration error and successive or global minimization of these bounds. The accuracy of these rules and the corresponding sparse grids (in dimension 2, 5 and 10) have been assessed for classical test functions.

The proposed 1D, (n/n+2) nested, interpolatory quadrature (LebConst-so, LebConst-go, LebInt - so, LebInt - go) have appeared to be equivalently good to those based on the classical Leja sequences. The efficiency of these methods with respect to less nested classical rules (Gauss-Legendre, Fejér second rule and Clenshaw-Curtis) is dependent

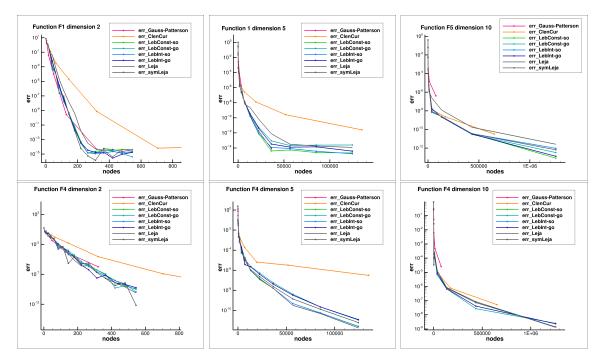


Figure 5: Test of sparse grid rules based for C^{∞} functions F_1 and F_5

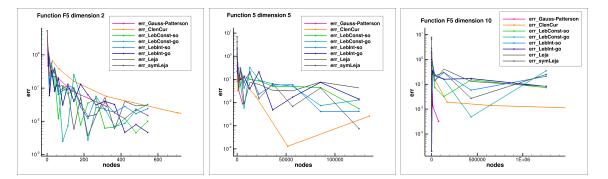


Figure 6: Test of sparse grid rules based for functions F_5 (C^1)

on the regularity of the function of interest (the lowest the regularity, the smallest the difference in quality).

When extending this work to nD Smolyak sparse grids using the "Smobol" tool of R.P. Dwight, once again, equivalent results have been obtained for rules derived from Leja sequences and from the proposed sequences. These sparse rules appeared to more efficient than Clenshaw-Curtis based sparse-grid for the integration of regular functions.

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