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New Methods for High-Dimensional Verified Quadrature

MARTIN BERZ and KYOKO MAKINO
Department of Physics and Astronomy, and National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, USA, e-mail: berz@pilot.msu.edu, makino@nscl.msu.edu

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Abstract. Conventional verified methods for integration often rely on the verified bounding of analytically derived remainder formulas for popular integration rules. We show that using the approach of Taylor models, it is possible to devise new methods for verified integration of high order and in many variables. Different from conventional schemes, they do not require an a-priori derivation of analytical error bounds, but the rigorous bounds are calculated automatically in parallel to the computation of the integral.

The performance of various schemes are compared for examples of up to order ten in up to eight variables. Computational expenses and tightness of the resulting bounds are compared with conventional methods.

1. Introduction

The verified solution of one- and higher dimensional integrals is one of the important problems using interval methods in numerics [1], [4], [5], [9]. The strategy is usually to derive formulas based on the evaluation of the function at a suitably chosen set of points x_i and the determination of a weighted average

$$I = \sum_{i=1}^{N} w_i \cdot f(x_i)$$

that approximates the integral of f over an interval $[X_1, X_2]$. By suitably choosing the points $x_i \in [X_1, X_2]$ as well as the weights w_i, it is possible to derive a formula for the local error of the method based on a higher derivative of f at an intermediate point ξ as

$$E = A \cdot f^{(k)}(\xi), \quad \text{where} \quad \xi \in [X_1, X_2].$$

The factor A depends on the method and usually includes a higher power of the width $X_2 - X_1$. Within the framework of interval analysis, it is then possible to determine bounds of E by evaluating the code for the derivative $f^{(k)}$, which is usually obtained from automatic differentiation, over the interval $[X_1, X_2]$ (see, for example, [10]).

In principle the method can be extended to higher orders, and also to several dimensions. However, especially schemes in higher dimensions and to high order can become rather cumbersome to derive and implement. Additional complications occur if the function f is sensitive to the dependency problem [8], in which case the evaluation of its error term via automatic differentiation, which requires even more arithmetic than f itself, can become difficult.

In the following, we use the Taylor model approach [2], [6], [7] for the computation of derivatives. This approach provides a local inclusion of a functional dependency within a tight band of constant width around a Taylor polynomial with floating point coefficients by merely evaluating f in Taylor model arithmetic. The method has the advantages that it is applicable in high order and in many variables, and that it provides error bounds that scale with a high power of the width of the domain bounds, while substantially reducing the dependency problem.

Given an n-th order Taylor model $(P_{n,f}, I_{n,f})$ of a function $f : [\vec{a}, \vec{b}] \subset R^v \to R$ consisting of the floating point Taylor polynomial $P_{n,f}$ and the remainder interval $I_{n,f}$ around the reference point $\vec{x}_0$, we can determine a Taylor model for the indefinite integral $\partial_i^{-1} f = \int f \, \mathrm{d}x_i$ with respect to the variable x_i. The Taylor polynomial part is obviously just given by $\int_0^{x_i} P_{n-1,f}(\vec{x}) \, \mathrm{d}x_i$ (here, $P_{n-1,f}$ is the Taylor polynomial of order $n-1$, i.e., the sum of all terms of order $\leq (n-1)$ in the polynomial $P_{n,f}$). Since the part of the Taylor polynomial $P_{n,f}$ that is of precise order n is $P_{n,f} - P_{n-1,f}$, remainder bounds can be obtained as $(B(P_{n,f} - P_{n-1,f}) + I_{n,f}) \cdot |B(x_i)|$, where $B(P_{n,f} - P_{n-1,f})$ is the bound of the polynomial of exact order n, and $|B(x_i)| = b_i - a_i$. We thus define the operator ∂_i^{-1} on the space of Taylor models as

$$\begin{aligned} \partial_i^{-1}(P_{n,f}, I_{n,f}) &= (P_{n,\partial^{-1}f}, I_{n,\partial^{-1}f}) \\ &= \left(\int_0^{x_i} P_{n-1,f}(\vec{x}) \, \mathrm{d}x_i, \; \big(B(P_{n,f} - P_{n-1,f}) + I_{n,f} \big) \cdot |B(x_i)| \right). \end{aligned} \tag{1.1}$$

With this definition, bounds for a definite integral over variable x_i from x_{il} to x_{iu} both in $[a_i, b_i]$, the domain of validity of the Taylor model of a function, can be obtained as

$$\int_{x_{il}}^{x_{iu}} f(\vec{x}) \, \mathrm{d}x_i \in \big(P_{n,\partial^{-1}f}(\vec{x}|_{x_i = x_{iu} - x_{i0}}) - P_{n,\partial^{-1}f}(\vec{x}|_{x_i = x_{il} - x_{i0}}), \; I_{n,\partial^{-1}f} \big). \tag{1.2}$$

This method has the following advantages:

1. There is no need to derive quadrature formulas with weights, support points x_i, and an explicit error formula.
2. High orders can be employed directly by just increasing the order of the Taylor model, limited only by computational resources.
3. Rather large dimensions are amenable by just increasing the dimensionality of the Taylor model, limited only by computational resources.

4. For complicated functions, the control of the dependency problem by the Taylor model approach [8] often results in significantly sharper bounds than those obtained through interval-Taylor methods, i.e. Taylor polynomials with interval coefficients.

In the following sections, we will study the approach for a variety of cases.

2. One-Dimensional Integrals

Utilizing the integral operation ∂^{-1} introduced in (1.1) and (1.2), it is possible to perform integration of functions of one or more variables. To increase the accuracy, the domain of the integral can be divided into sub-domains within which the function is represented by local Taylor models. To obtain the total integral, each of the local Taylor models is integrated, which requires the application of the operators ∂_i^{-1}, subsequent evaluations of polynomials as well as adding the interval bounds. Accuracy can be controlled both by adjustment of the width of the local domains as well as of the order n. In practice it is quite straightforward to operate with orders of ten or higher, and as a consequence the resulting accuracy is not only guaranteed, but the method is also very efficient.

We compare this method with a variety of other verified integration schemes, beginning with the straightforward step rule, in which upper and lower bounds of the function are obtained over subintervals by mere interval evaluation. We also employ the conventional trapezoidal rule as well as the Simpson 1/3 rule, including verification through their error formulas, which requires the bounding of the second and the fourth derivatives of the integrand, respectively.

As an example, we study the definite integral of a one dimensional function

$$\int_0^1 \frac{4}{1+x^2}\,\mathrm{d}x,$$

the value of which is known to be π. Table 1 summarizes the resulting estimates with various divisions of the domain of the integral. The step rule covering the whole domain by one interval gives an enclosure which is too wide to be useful. To increase the sharpness of the enclosure, the whole domain is divided into many smaller intervals. The trapezoidal and Simpson rules reach accuracies of about 10^{-6} and 10^{-15} with a subdivision into 1000 intervals. On the other hand, the fifth- and tenth order Taylor model integrations reach about 10^{-7} and 10^{-14} verified accuracy with only 16 subdivisions of the interval. We also show the non-verified estimates of the Monte-Carlo approach, which because of its simplicity will be used below for high-dimensional problems.

Table 1. Bound estimates of $\int_0^1 4\,/\,(1+x^2)\,dx$.

Analytical Answer		$\pi \approx$ 3.1415926535897
Step Rule with Verification		
Subdivisions		Bound
1		[2.0000000000000 , 4.0000000000000]
10		[3.0399259889071 , 3.2399259889071]
100		[3.1315759869231 , 3.1515759869231]
1000		[3.1405924869231 , 3.1425924869231]
Trapezoidal Rule with Verification		
Subdivisions		Bound
1		[0.5000000000000 , 3.6666666666666]
10		[3.1403914418783 , 3.1425703033023]
100		[3.1415915590081 , 3.1415937257970]
1000		[3.1415926525053 , 3.1415926546720]
Simpson 1/3 Rule with Verification		
Subdivisions		Bound
1		[2.5666666666666 , 3.5291666666666]
10		[3.1415909377638 , 3.1415944278590]
100		[3.1415926535726 , 3.1415926536069]
1000		[3.1415926535897 , 3.1415926535897]
Monte-Carlo Method (not verified)		
Sampling Points		Estimate
1		3.0644927519710
100		3.1750796498765
10000		3.1472009776816
1000000		3.1401270041329
Taylor Model Method		
Order	Subdivisions	Bound
5	1	[3.0231893333333 , 8.5807786666666]
	4	[3.1415363229415 , 3.1416629536292]
	16	[3.1415926101614 , 3.1415926980786]
10	1	[-2.1984010266006 , 3.2113963175267]
	4	[3.1415926519535 , 3.1415926546870]
	16	[3.1415926535897 , 3.1415926535897]

3. Multidimensional Integrals

3.1. A Three-Dimensional Example

The first example is a somewhat randomly chosen complicated function of three variables:

$$\begin{aligned} f(x,y,z) &= \frac{4\tan(3y)}{3x + x\sqrt{6x/(56-7x)}} - 120 - 2x \\ &\quad - 7z(1+2y) - \sinh\left(\frac{1}{2} + \frac{6y}{8y+7}\right) \\ &\quad + \frac{(3y+13)^2}{3z} - 20z(2z-5) + \frac{5x\tanh(0.9z)}{\sqrt{5y}} - 20y\sin(3z). \end{aligned}$$

Integration was performed over the range $[3/4, 5/4] \times [3/4, 5/4] \times [3/4, 5/4]$. In Table 2, we compare the performance of the step rule and the trapezoidal rule, which because of the complexity of the derivation of a remainder formula was not verified, with the computation using Taylor models of order five and ten, requiring a total of 56 and 286 coefficients respectively. Again, various subdivisions of the domain were performed.

One observes that the use of just one Taylor model of order ten to cover the entire domain yields a sharpness comparable to that of the use of $16^3 = 4096$ subintervals in the trapezoidal rule. Increasing the subdivisions to $8^3 = 512$ subintervals in the Taylor model approach yields 10 digit accuracy, which would be reached by the trapezoidal rule only at an estimated 10^{10} subintervals.

3.2. Examples in Four, Six, and Eight Dimensions

We now concentrate on the determination of integrals of high dimensions. With conventional methods, these are often very difficult to treat: On the one hand, one needs high order for the sake of staying within a manageable number of subdivisions per dimension: On the other hand, it is quite complicated to derive error formulas for such high-order multidimensional cases. Compared to this predicament, in the Taylor model approach, there is no increased theoretical effort, and high orders and many dimensions can still be treated with reasonable effort.

In order to benchmark the various algorithms, we construct multidimensional integrals whose analytical values are known. They are based on the following double definite integral found in [3].

$$\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}} \frac{\sin y\sqrt{1-k^2\sin^2 x\sin^2 y}}{1-k^2\sin^2 y}\,\mathrm{d}x\,\mathrm{d}y = \frac{\pi}{2\sqrt{1-k^2}}.$$

In order to assess the performance of algorithms in higher dimensionalities, we use this integral to construct four-, six-, and eight dimensional integrals with

Table 2. Bound estimates of a three dimensional integral.

Step Rule with Verification		
Subdivisions		Bound
1		[-9.43480535560 , 11.84444223367]
4^3		[-2.37821189737 , 2.81357566502]
16^3		[-0.49305930286 , 0.80296307748]
64^3		[-0.01095827969 , 0.31301380623]
Trapezoidal Rule		
Subdivisions		Estimate
1		0.48657769881
4^3		0.17278422284
16^3		0.15214575522
64^3		0.15085237990
Monte-Carlo Method		
Sampling Points		Estimate
1		0.97878177127
100		0.00229810669
10000		0.14778035060
1000000		0.15154470170
Taylor Model Method		
Order	Subdivisions	Bound
5	1	[0.08429328162 , 0.22934882912]
	2^3	[0.14823776771 , 0.15294164469]
	4^3	[0.15068701132 , 0.15084227488]
	8^3	[0.15076370507 , 0.15076856317]
10	1	[0.14602544640 , 0.15436708172]
	2^3	[0.15075284566 , 0.15077186956]
	4^3	[0.15076611865 , 0.15076615436]
	8^3	[0.15076614172 , 0.15076614177]

known value to serve as test cases. As a first step, we obtain the four dimensional integral

$$\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}} \left(\frac{\sin y\sqrt{1-k^2\sin^2 x\sin^2 y}}{1-k^2\sin^2 y} + \frac{\sin w\sqrt{1-k^2\sin^2 z\sin^2 w}}{1-k^2\sin^2 w}\right) \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}w,$$

Table 3. Bound estimates of a four dimensional integral.

Analytical Answer		$\pi^3 / (4\sqrt{1-k^2}) \approx$ 8.170871339 for $k^2 = 0.1$
Step Rule with Verification		
Subdivisions		Bound
1		[0.707312958E-15, 13.529040421]
4^4		[6.344461569 , 9.814754327]
16^4		[7.730435550 , 8.599902240]
Trapezoidal Rule		
Subdivisions		Estimate
1		6.590953776
4^4		8.071117282
16^4		8.164644803
Monte-Carlo Method		
Sampling Points		Estimate
1		10.718624190
100		7.850754773
10000		8.197884624
1000000		8.176000177
Taylor Model Method		
Order	Subdivisions	Bound
5	1	[7.133074468 , 9.204470869]
	2^4	[8.148975985 , 8.192531932]
	4^4	[8.170404693 , 8.171334032]
10	1	[8.139359412 , 8.205450807]
	2^4	[8.170848978 , 8.170894025]
	4^4	[8.170871325 , 8.170871354]

which is to have the value of $\pi^3 / (4\sqrt{1-k^2})$. Attempting to solve the integral with the quadrature engines in Mathematica and Maple fails. The definite integral for $k^2 = 0.1$ is approximately 8.170871339259325. Similar to before, computations are made to obtain the bounds with the step rule and the Taylor model method as shown in Table 3. Apparently all estimates obtained by the Taylor model approach yield correct inclusions, and in case of tenth order Taylor models the sharpness reaches eight significant digits with only four subdivisions per dimension, corresponding to a grid size of $\pi / 8$. It is also apparent that the accuracy increases by roughly three orders of magnitude each time the grid size is reduced by a factor of two,

Table 4. Bound estimates of a six dimensional integral.

Analytical Answer		$3\pi^5 / (32\sqrt{1-k^2}) \approx$ 30.24122539 for $k^2 = 0.1$
Step Rule with Verification		
Subdivisions		Bound
1		[0.261783715E-14, 50.07235383]
2^6		[16.12883946 , 41.65021086]
4^6		[23.48149718 , 36.32540343]
Trapezoidal Rule		
Subdivisions		Estimate
1		24.39378990
2^6		28.75885830
4^6		29.87202549
Monte-Carlo Method		
Sampling Points		Estimate
1		32.08739916
100		29.38558165
10000		30.28333639
1000000		30.23656210
Taylor Model Method		
Order	Subdivisions	Bound
5	1	[26.40023368 , 34.06668232]
	2^6	[30.16018846 , 30.32139345]
	4^6	[30.23949829 , 30.24293787]
10	1	[30.12459655 , 30.36920752]
	2^6	[30.24114263 , 30.24130936]
	4^6	[30.24122534 , 30.24122545]

corresponding to the expected decrease of the error with the tenth order of the grid size.

In a similar manner, the integral problem is extended to the six dimensional and the eight dimensional cases, where the question of computer resources becomes non-negligible even for the evaluation with the simple trapezoidal rule without any error verification. The results are shown in Table 4 and Table 5, where we find the tenth order Taylor model computation without any domain division already gives a remarkably good bound estimate.

Table 5. Bound estimates of an eight dimensional integral.

Analytical Answer		$\pi^7 / (32\sqrt{1-k^2}) \approx$ 99.48964376 for $k^2 = 0.1$
Step Rule with Verification		
Subdivisions		Bound
1		[0.861233904E-14, 164.73144125]
2^8		[53.06175498 , 137.02370147]
4^8		[77.25102931 , 119.50578720]
Trapezoidal Rule		
Subdivisions		Estimate
1		80.25235205
2^8		94.61285151
4^8		98.27502476
Monte-Carlo Method		
Sampling Points		Estimate
1		72.40666558
100		95.61473748
10000		99.86545191
1000000		99.50324225
Taylor Model Method		
Order	Subdivisions	Bound
5	1	[86.85328752 , 112.07489259]
	2^8	[99.22304294 , 99.75338610]
	4^8	[99.48396181 , 99.49527757]
10	1	[99.10595024 , 99.91068808]
	2^8	[99.48937149 , 99.48991998]
	4^8	[99.48964358 , 99.48964393]

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