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Convergence analysis and adaptive strategy for the certified quadrature over a set defined by inequalities

Alexandre Goldsztejn [a,*], Jorge Cruz [b], Elsa Carvalho [b]

[a] CNRS, Laboratoire d'Informatique de Nantes Atlantique, Nantes, France

[b] CENTRIA, Departamento de Informática, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal

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ABSTRACT

This paper investigates the sufficient conditions for the asymptotic convergence of a generic branch and prune algorithm dedicated to the verified quadrature of a function in several variables. Quadrature over domains defined by inequalities, and adaptive meshing strategies are in the scope of this analysis. The framework is instantiated using certified quadrature methods based on Taylor models (i.e. Taylor approximations with rigorously bounded remainder), and reported experiments confirmed the analysis. They also show that the performances of the instantiated algorithm are comparable with current methods for certified quadrature.

1. Introduction

In the present paper, we investigate the asymptotic convergence of an adaptive splitting algorithm dedicated to rigorously enclosing the integral

$$\int_{\Omega} f(\mathbf{x})d\mathbf{x} \tag{1}$$

where $\Omega = \{\mathbf{x} \in [\mathbf{x}^{\text{Init}}] : g(\mathbf{x}) \leq 0\}$ and $[\mathbf{x}^{\text{Init}}]$ a bounded box (boldface symbols represent vectors, bracketed symbols represent intervals, e.g. $[\mathbf{x}] = ([x_1], \ldots, [x_n])$ is a box, and $d\mathbf{x}$ stands for $dx_1 \ldots dx_n$). The studied branch and prune algorithm applies some arbitrary certified quadrature methods to subdomains that are recursively split. Since certified quadrature methods are more and more accurate as the domain size decreases, the overall algorithm is expected to converge asymptotically to the exact quadrature. Such convergence study was already carried out in some restricted case, see e.g. [1] where the asymptotic convergence was proved when a regular meshing with Taylor model based certified quadrature is applied to the quadrature over a box domain. This paper generalizes the convergence analysis by providing sufficient conditions enforcing the branch and prune algorithm asymptotical convergence. These sufficient conditions apply to generic quadrature methods, handle quadrature domains defined by inequalities and adaptive meshing strategies.

Using a branch and prune algorithm clearly presents pros and cons with respect to regular meshing, whose compromise is analyzed in this paper: on the one hand, when a box is split the integral of the function of the resulting sub-boxes is computed, and thus the integral that has been computed for the initial box is useless. This leads to repeated useless computations, doubling the number of calls to the generic integration procedure in the worst case (since the number of nodes in a binary tree is at most twice the number of it leaves). On the other hand, the branch and prune algorithm presents

* Corresponding author. Tel.: +33 678049487.
E-mail addresses: Alexandre.Goldsztejn@univ-nantes.fr (A. Goldsztejn), jc@di.fct.unl.pt (J. Cruz), elsac@uma.pt (E. Carvalho).

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the key advantage of allowing adaptive mesh refinement,[1] which allows both reducing the overall computational effort and improving the final enclosure (since oversplitting leads to unnecessary computations and rounding errors).

Interval analysis is introduced in Section 2 with emphasis on convergence properties. Generic quadrature inclusion functions are defined in Section 3, together with their properties related to asymptotic convergence. The branch and prune algorithm dedicated to the certified enclosure of (1) is described in Section 4. The convergence analysis of this branch and prune algorithm is investigated theoretically in Section 5 together with its rate of convergence. Finally, the framework is instantiated with Taylor model based quadrature methods: Although other methods allow computing certified quadrature (e.g. [3–5]), Taylor models are efficient and have good asymptotical convergence properties. Experiments on standard benchmarks from the literature [6–9] are presented in Section 6 to support this convergence analysis. A detailed comparison is reported with respect to several algorithms [6,10,9] dedicated to the certified enclosure of (1). Finally, Taylor models are presented in the Appendix, with emphasis on their usage to certified quadrature and their convergence.

2. Interval analysis

Interval analysis is a modern branch of numerical analysis that was born in the 60's. It consists of computing with intervals of reals instead of reals, providing a framework for handling uncertainties and verified computations (see [11–15] for a survey). Section 2.1 presents the basic definitions related to interval extensions, and Section 2.2 some properties related to their convergence.

2.1. Interval extensions

An interval is a connected subset of $\mathbb{R}$. Intervals are denoted by bracketed symbols, e.g. $[x] \subseteq \mathbb{R}$. When no confusion is possible, lower an upper bounds of an interval $[x]$ are denoted by $\underline{x} \in \mathbb{R}$ and $\overline{x} \in \mathbb{R}$, with $\underline{x} \leq \overline{x}$, i.e. $[x] = [\underline{x}, \overline{x}] = \{x \in \mathbb{R} : \underline{x} \leq x \leq \overline{x}\}$. Furthermore, a real number x will be identified with the degenerated interval $[x, x]$. The width, midpoint and magnitude of an interval are respectively defined by $\operatorname{wid}[x] := \overline{x} - \underline{x}$, $\operatorname{mid}[x] := 0.5(\overline{x} + \underline{x})$, $\operatorname{mag}[x] := \max\{|\underline{x}|, |\overline{x}|\}$.

There are two equivalent ways of defining interval vectors. On the one hand, being given two vectors $\underline{\mathbf{x}} \leq \overline{\mathbf{x}} \in \mathbb{R}^n$ (where the inequality is defined componentwise), an interval of vectors is obtained by considering

$$[\mathbf{x}] := \{\mathbf{x} \in \mathbb{R}^n : \underline{\mathbf{x}} \leq \mathbf{x} \leq \overline{\mathbf{x}}\}. \tag{2}$$

On the other hand, being given intervals $[x_i] \in \mathbb{IR}$ for $i \in \{1, \ldots, n\}$, a vector of intervals is obtained by considering

$$[\mathbf{x}] := \{\mathbf{x} \in \mathbb{R}^n : \forall i \in \{1, \ldots, n\}, x_i \in [x_i]\}. \tag{3}$$

These two definitions are obviously equivalent following the notational convention $\underline{\mathbf{x}} = (\underline{x}_i)$, $\overline{\mathbf{x}} = (\overline{x}_i)$ and $[x_i] = [\underline{x}_i, \overline{x}_i]$, and will be used indifferently. The width, volume and midpoint of an interval vector are respectively defined by $\operatorname{wid}[\mathbf{x}] := \max_i \operatorname{wid}[x_i] \in \mathbb{R}$, $\operatorname{vol}[\mathbf{x}] := \prod_i \operatorname{wid}[x_i] \in \mathbb{R}$ and $\operatorname{mid}[\mathbf{x}] := 0.5(\overline{\mathbf{x}} + \underline{\mathbf{x}}) \in \mathbb{R}^n$.

Operations $\circ \in \{+, \times, -, \div\}$ are extended to intervals in the following way:

$$[x] \circ [y] := \{x \circ y : x \in [x], y \in [y]\}. \tag{4}$$

The division is defined for intervals $[\underline{y}, \overline{y}]$ that do not contain zero. Unary elementary functions $f(x)$ (like exp, ln, sin, etc.) are also extended to intervals similarly:

$$f([x]) = \{f(x) : x \in [x]\}. \tag{5}$$

All these elementary interval extensions form the interval arithmetic. As real numbers are identified to degenerated intervals, the interval arithmetic actually generalizes the real arithmetic, and mixed operations like $1 + [1, 2] = [2, 3]$ are interpreted using (4).

An interval function $[f] : \mathbb{IR}^n \longrightarrow \mathbb{IR}$ is an interval extension of the real function $f : D \subseteq \mathbb{R}^n \longrightarrow \mathbb{R}$ if for all $[\mathbf{x}] \in \mathbb{IR}^n$ we have $[f]([\mathbf{x}]) \supseteq \{f(\mathbf{x}) : \mathbf{x} \in D \cap [\mathbf{x}]\}$. Thus interval extensions allow computing enclosures of real functions range over boxes. So called natural interval extensions of a function are obtained by evaluating an expression of this function for interval arguments using the interval arithmetic.

Example 1. Let $f(x, y) = x(y - x)$. The interval function $[f]([x], [y]) = [x]([y] - [x])$ is the natural interval extension of f. Hence for example

$$[f]([0, 1], [-1, 1]) = [-2, 1] \supseteq \{f(x, y) : x \in [0, 1], y \in [-1, 1]\}. \tag{6}$$

Note that the exact range is $f([0, 1], [-1, 1]) = \left[-2, \frac{1}{4}\right]$, and the natural interval extension is thus pessimistic. One central issue of interval analysis is to fight this pessimism introduced by the interval evaluation of a function.

There are other interval extensions, in particular the mean-value interval extension which uses the natural extension of the derivatives to try improving the enclosure. See [13] for details. Throughout the paper, we suppose that involved interval extensions are inclusion isotone (i.e. $[\mathbf{x}'] \subseteq [\mathbf{x}]$ implies $[f]([\mathbf{x}']) \subseteq [f]([\mathbf{x}])$), which generally holds.

[1] Such adaptive strategies are known to be of critical importance also in the context of non verified quadrature, see e.g. [2]