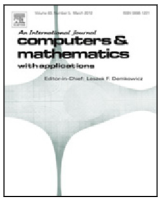
ARTICLE IN PRESS

Computers and Mathematics with Applications ■ (■■■■) ■■■–■■■

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa



Rigorous cubical approximation and persistent homology of continuous functions

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ARTICLE INFO

Article history:
Received 12 October 2016
Received in revised form 5 June 2017
Accepted 20 November 2017
Available online xxxx

Keywords:
Rigorous approximation of functions
Rigorous arithmetic
Constructive version of simplex approximation theorem
Persistent homology
Rigorous computations

ABSTRACT

The interaction between discrete and continuous mathematics lies at the heart of many fundamental problems in applied mathematics and computational sciences. In this paper we discuss the problem of discretizing vector-valued functions defined on finite-dimensional Euclidean spaces in such a way that the discretization error is bounded by a pre-specified small constant. While the approximation scheme has a number of potential applications, we consider its usefulness in the context of computational homology. More precisely, we demonstrate that our approximation procedure can be used to rigorously compute the persistent homology of the original continuous function on a compact domain, up to small explicitly known and verified errors. In contrast to other work in this area, our approach requires minimal smoothness assumptions on the underlying function.

1. Introduction

In many applied situations it is necessary to replace a given smooth function by a discretized version which in some sense is close to the given original mapping. In this paper we discuss a number of algorithms for approximating a continuous function $f : D \to \mathbb{R}^m$, defined on a compact rectangular domain $D \subset \mathbb{R}^n$, using piecewise constant functions. In order to achieve approximations with mathematically verified approximation bounds, our approach relies on the use of rigorous computer arithmetic. One such example is interval arithmetic [1], and it will form the foundation of the algorithms described in the present paper. However, our approach can also be used with any other rigorous computer arithmetic which provides rigorous enclosures of function values. For example, our algorithms can readily be adapted to employ alternative tools such as affine arithmetic [2], generalized interval arithmetic [3], or in fact, any other rigorous arithmetic capable of providing range enclosures.

Upon successful completion, the algorithms presented in this paper will return a decomposition of the rectangular domain D into a collection of compact n-dimensional rectangles, any two of which only intersect in a subset of their topological boundaries. Furthermore, each rectangle R in the collection is assigned a value $val(R)$ in $\mathbb{R}^m$. The approximating function $\square f$ is then defined in the following way. For every rectangle R in the constructed decomposition, the function value of $\square f$ in the interior of R is given by $val(R)$. On the other hand, if $x \in D$ lies in the intersection of k rectangles $R_1, \ldots, R_k$, then we define $\square f(x) = \min_{i=1,\ldots,k} val(R_i)$. In this way, the decomposition of D produced upon successful completion of the algorithm gives rise to a lower semi-continuous piecewise constant approximation $\square f$ of the given continuous function f. We will see later that the algorithm in fact guarantees the inequality

$$\|f - \square f\|_\infty < \varepsilon \,, \qquad \text{where } \varepsilon > 0 \text{ denotes the input parameter of the algorithm,}$$

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https://doi.org/10.1016/j.camwa.2017.11.027
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Please cite this article in press as: P. Dłotko, T. Wanner, Rigorous cubical approximation and persistent homology of continuous functions, Computers and Mathematics with Applications (2017), https://doi.org/10.1016/j.camwa.2017.11.027.

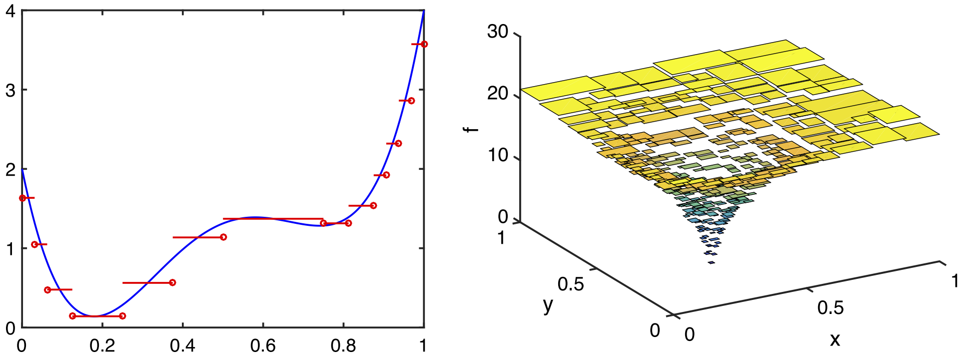

Fig. 1. Sample approximating functions $\square f$. The left image is for the one-dimensional function $f(x) = 2 - 25x + 108x^2 - 162x^3 + 81x^4$ on the interval $D = [0, 1]$, and with approximation parameter $\varepsilon = 1/2$. The function f is shown in blue, while its approximation $\square f$ is depicted in red. Red circles indicate the function values at the points in D which are contained in more than one intervals of the final decomposition. The right panel shows an approximation for the Ackley function with $\varepsilon = 2$.

and where $\|\cdot\|_\infty$ denotes the usual maximum norm. This procedure is illustrated in the two panels of Fig. 1. In the left panel, the approximating function $\square f$ is shown for the one-dimensional function $f(x) = 2 - 25x + 108x^2 - 162x^3 + 81x^4$ on the interval $D = [0, 1]$, and with approximation parameter $\varepsilon = 1/2$. The right panel contains the approximation for the so-called Ackley function, which is one of the standard test functions in nonlinear optimization and which will be discussed in more detail later in this paper.

The approximation algorithms presented in this paper can in principle be applied in a number of situations. For example, in the context of global optimization they allow one to rigorously narrow down the search for global minima or maxima of a real-valued function, as can easily be seen in the examples of Fig. 1. Rather than pursuing such applications, we confine ourselves to the computation of the persistent homology of a function. One-dimensional persistent homology was introduced in [4], and since then has become one of the main topological tools in the applied sciences for studying the shape of functions or spaces. Its popularity can be attributed to a variety of factors:

- Persistent homology provides quantitative information about the object of interest, including information about its shape,
- the obtained information is both metric and coordinate free, and
- the information is preserved under continuous deformations, e.g., it is invariant with respect to isometries.
- Persistence captures topological information at different scales,
- it is robust with respect to the influences of random noise, and
- efficient algorithms are available for its computation.

At present, persistent homology can only be determined algorithmically for the case of scalar-valued functions, i.e., only one-dimensional persistence is amenable to a computational treatment. For this, one needs to find a suitable filtration of a finite cell complex, and the results of this paper will enable its efficient construction. Due to deep results from quiver theory [5], there are no finite invariants which completely characterize multi-dimensional persistent homology. Nevertheless, there are many groups working on providing partial invariants for multi-dimensional persistent homology that can be used in practice.

The algorithms presented in this paper for the case of functions $f : D \subset \mathbb{R}^n \to \mathbb{R}^m$ provide discretizations of f with rigorous error bounds. These discretizations can immediately be used in the computation of one-dimensional persistent homology, i.e., in the scalar-valued case $m = 1$. We would like to point out, however, that the approximations can potentially also be used in the context of recently developed algorithms which compute partial invariants of multi-dimensional persistent homology. In order to specifically accommodate the computation of persistent homology, we consider specific approximations in which, in addition to the rectangular decomposition of the domain D, we also keep track of all the intersections of the rectangles in the decomposition. This is achieved by constructing a weighted cell complex which will later be used to compute persistent homology or some invariants of multi-dimensional persistent homology.

Approximating continuous functions is a part of the classical simplicial approximation theorem [6]. However, we are not aware of any attempts to create lower semi-continuous approximations of continuous functions using rigorous computer arithmetic. In the context of differentiable functions, the work [7] comes close in spirit to the present paper. The authors use a generalization of quad-trees and oct-trees to compute compatible cellular decompositions for level sets of a given differentiable function. Then, after computing the generators of the associated homology groups at each level of the filtration, together with their inclusions, they obtain the persistent homology of a differentiable function. It is worth mentioning that through the computation of the persistence of inclusions between two fixed level sets, the authors of [7] obtain an exact persistence result for the chosen levels. Similar idea to compute standard persistent homology was used in [8]. This, however,

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