Robustness of Zero Sets: Implementation

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Abstract

Robustness of zero of a continuous map $f\colon X \to \mathbb{R}^n$ is the maximal $r > 0$ such that each $g\colon X \to \mathbb{R}^n$ with $\|f-g\|_\infty \le r$ has a zero. We develop and implement an efficient algorithm approximating the robustness of zero and present computational experiments.

The main ingredient is an algorithm for deciding the topological extension problem based on computing cohomological *obstructions* to extendability and their robustness.

1 Introduction

Statement of the result. We describe an algorithm for detecting zeros of vector valued functions $f : X \to \mathbb{R}^n$ on a compact space X and for approximating the *robustness* of zero, that is, a maximal number $r > 0$ such that every continuous $g : X \to \mathbb{R}^n$ satisfying $\|g - f\| \le r$ has a zero. By $\|f\|$ we denote the max norm of f, that is, $\max_{x\in X} |f(x)|$ where $|\cdot|$ is a fixed ℓ_p norm in $\mathbb{R}^n$. Nontrivial cases happen if $\dim X \ge n$, as otherwise arbitrarily small perturbations of f avoid zero.

For computer representation we assume that the space X is a simplicial complex. Then the map $f\colon X \to \mathbb{R}^n$ is specified by its values on the vertices and by a value $\alpha > 0$ such that $|f(x) - f(y)| \le \alpha$ for arbitrary points x and y of any simplex of X. In an alternative setting we might assume that the function f is *simplexwise linear*,[1] but we preferred to emphasize that the precise knowledge of f is not needed (at the cost of slightly worse approximation guarantees).

The main motivation for the theoretical part of this paper was to give a rigorous analysis of an implementation that is tailored for real instances. We perceive the contribution of this paper as follows.

- *Feasibility.* Our algorithm is designed to avoid any time-costly numerical computations. Unlike the algorithm of [3], we need neither barycentric subdivisions nor convex optimization.
- *Persistent cohomology computations over integers.* As an auxiliary tool, we need to extract certain information from a persistent module $H^*(X_0;\mathbb{Z}) \to H^*(X_1;\mathbb{Z}) \to \dots$ with integral coefficients. To that end, we adapted the Chen's and Kerber's matrix reduction algorithm "with a twist" [2].
- *Implementation.* Our implementation is available online[2] and several computational experiments are presented in our preprint [4].

Methods and the outline of the algorithm. The main tools come from the field of *computational homotopy theory.* In [3] we showed that any function $f\colon X \to \mathbb{R}^n$ on a compact domain X, has an r-robust zero if and only if the map

$$f|_{A(r)} : A(r) \to \mathbb{R}^n \setminus \{0\} \text{ where } A(r) := \{x \in X : |f(x)| \ge r\} \tag{1}$$

cannot be extended to a map $X \to \mathbb{R}^n \setminus \{0\}$. After replacing f by the map $x \mapsto f(x)/|f(x)|$, we can equivalently replace $\mathbb{R}^n \setminus \{0\}$ by S^{n-1}. This extension problem is the core of our algorithm for approximating robustness, outlined as follows.

A. First, we discretize the continuous input, that is, convert the spaces $A(r)$ into simplicial complexes A_r. Unlike in [3], we do not aim at having homotopy equivalence $A(r) \simeq A_r$ which requires additional subdivisions and thus increases the computing time heavily. For obtaining approximate results it is sufficient to have a relation of the form $A(r-\alpha) \supseteq A_r \supseteq A(r+\alpha)$ for some reasonably small α. Such a relation can be achieved without introducing additional subdivisions while using the simplexwise Lipschitz property of f.

   We also identify some smallest value r_0 such that the restriction of f to A_{r_0} can be easily *discretized.* A simple combinatorial procedure finds a simplicial map f' from A_{r_0} to the sphere such that f' is homotopic to f as map from A_{r_0} to the $(n-1)$-sphere.

B. In the second step, we do pure computational homotopy theory. Namely, for a previously obtained sequence of simplicial complexes $X \supseteq$

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[1] That is, on every simplex it linearly interpolates the values on the vertices. Such functions defined on sufficiently fine subdivision of X can approximate any continuous map $X \to \mathbb{R}^n$ arbitrarily well.

[2] www.cs.cas.cz/~franek/rob-sat

$A_0 \supseteq A_1 \supseteq \ldots \supseteq A_h = \emptyset$ and a simplicial sphere-valued map f' we ask for robustness of non-extendability of f' defined as follows.

Definition 1 *Let $X \supseteq A_0 \supseteq A_1 \supseteq \ldots$ be a filtration and $f' : A_0 \to S^{n-1}$ a sphere-valued map that cannot be extended to all of X. The* robustness of non-extendability of f' from $(A_i)_{i\geq 0}$ to X *is the smallest index i such that $f'|_{A_i}$ cannot be extended to the whole of X.*

2 Discretizing the geometry of the zero sets of perturbations

Definition 2 *A* continuous filtration *of spaces is a family $(A_r)_{r\in\mathbb{R}}$ such that $A_r \supseteq A_s$ whenever $r \leq s$.*

A continuous filtration $(A_r)_{r\in\mathbb{R}}$ is called step-like *whenever there exists a sequence of numbers $-\infty =: r_{-1} < r_0 \leq r_1 \leq r_2 \leq \ldots \leq r_k$ such that for any $r, s \in (r_i, r_{i+1}]$ holds $A_r = A_s$ for all i.*

Note that any such step-like continuous filtration is determined by the sequence of reals $(r_i)_i$ and the filtration $A_0 \supseteq A_1 \supseteq \ldots \supseteq A_k$ where each A_i denotes A_{r_i}.

Definition 3 *Continuous filtrations $(A_r)_r$ and $(B_r)_r$ are called α-interleaved whenever $B_{r+\alpha} \subseteq A_r$ and $A_{r+\alpha} \subseteq B_r$ for each $r \in \mathbb{R}$.*

Definition 4 *Let $f\colon X \to \mathbb{R}^n$ be a continuous map on a simplicial complex X and let $|\cdot|$ be a norm on $\mathbb{R}^n$.*

1. *Then by A_r we denote the subcomplex of X spanned by the vertices v of X with $|f(v)| \geq r$.*
2. *By $A(r)$ we denote the subspace of X defined by $A(r) = \{x \in X : |f(x)| \geq r\}$.*
3. *We say that f is* simplexwise α-Lipschitz *whenever $|f(x) - f(y)| \leq \alpha$ for each pair of points $x, y \in \Delta$ of any simplex $\Delta \in X$.*

Spaces A_r form a step-like filtration where the steps occur for each r equal to $|f(v)|$ for some vertex v of X.

We will represent the sphere S^{n-1} via a simplicial complex Σ^{n-1}, the boundary of the n-dimensional cros-polytope. Denoting $e_1, \ldots, e_n$ the canonical basis vectors of $\mathbb{R}^n$, simplices of Σ^{n-1} are all those subsets of $\{\pm e_i \,|\, i = 1, \ldots, n\}$ that do not contain a pair of antipodal vectors $\{e_i, -e_i\}$.

Theorem 1 *Let $f\colon X \to \mathbb{R}^n$ be a simplexwise α-Lipschitz map for some constant $\alpha > 0$. Then the following holds:*

1. *The continuous filtrations $(A_r)_{r\in\mathbb{R}}$ and $A(r)_{r\in\mathbb{R}}$ are α-interleaved.*
2. *For any ℓ_p norm once $r > \alpha n^{1/p}/2$, the mapping of vertices*

$$\begin{aligned} f' : V(A_r) &\to V(\Sigma^{n-1}) \\ v &\mapsto \operatorname{sgn}\big(f(v)_{i^*}\big) e_{i^*} \\ \text{where } \; i^* &= \operatorname*{argmax}_{i=1,\ldots,n} \big|f(v)_i\big| \end{aligned} \tag{2}$$

   defines a simplicial map $f'\colon A_r \to \Sigma^{n-1}$ (that is, it maps simplices to simplices).

   Moreover, $f'\colon A_r \to \Sigma^{n-1} \subseteq \mathbb{R}^n \setminus \{0\}$ is homotopic to $f|_{A_r}\colon A \to \mathbb{R}^n \setminus \{0\}$ once $r > \alpha n^{1/p}$.

The simplicial map $f'\colon A \to \Sigma^{n-1}$ as above will be called the *simplicial approximation of $f|_A$*.

3 The algorithm using an oracle for robustness of non-extendability.

Now it is convenient to state the algorithm for approximating robustness of zero, given an oracle for computing or bounding from below the robustness of non-extendability.

A. (a) Label the set of real values $\{|f(v)|\colon v \in V(X) \text{ such that } |f(v)| \geq \alpha n^{1/p}\}$ by $\{r_0, r_1, \ldots, r_h\}$ for some integer $h \geq 0$.

   (b) For any simplex $\Delta \in X$ compute its filtration value $r(\Delta)$ by

   $$r(\Delta) := \min_{v \text{ vertex of } \Delta} |f(v)|.$$

   This yields a filtration $A_0 = A_{r_0} \supseteq \ldots \supseteq A_h = A_{r_h}$ that together with the values $r_0, \ldots, r_h$ determines the step-like continuous filtration $(A_r)_{r\in\mathbb{R}}$ from Definition 4.

   (c) For vertices v of X with $|f(v)| \geq r_0$ compute $f'(v)$ defined by (2).

B. Use oracle to compute or bound from below the robustness i^* of non-extendability of f' from $(A_i)_{i\geq 0}$ to X.

   (a) Once $i^* \geq j$ and $j > 0$, output "robustness of zero is at least $r_j - \alpha$."

   (b) Once also $i^* \leq j$, output "robustness of zero is at most $r_j + \alpha$."

Using the fact that the nonextendability of (1) is equivalent to the existence of an r-robust zero combined with Theorem 1, we can easily prove that the above algorithm outputs a correct statement.

4 Robustness of obstructions to extendability.

Here we review the basic facts from obstruction theory. $X^{(k)}$ will always refer to the k-skeleton of X, the sub-complex spanned by simplices of dimension

$\leq k$. Any map $f : A \to S^{n-1}$ can be extended to $A \cup X^{(n-1)} \to S^{n-1}$ by the connectivity of the sphere. At some point of our extension process we need to work on the level of cocycles. Also our implementation operates fully on the level of cochains and cocycles, hence we stick to that point of view for most of the exposition as well. Let $z \in Z^{n-1}(\Sigma^{n-1}, \mathbb{Z})$ be a fixed representative of the generator of $H^{n-1}(\Sigma^{n-1}; \mathbb{Z})$. We will use the following facts:

Proposition 2 *Let $f\colon A \to \Sigma^{n-1}$ be simplicial, $X \supseteq A$, and $y := f^\sharp(z) \in Z^{n-1}(A; \mathbb{Z})$. Then the following holds:*

1. *Any map $h\colon A \cup X^{(n-1)} \to \Sigma^{n-1}$ extendable to $X^{(n)}$ such that $h|_A = f$ can be described up to a homotopy stationary on A by a cocycle $x \in Z^{n-1}(X; \mathbb{Z})$ such that $x|_A = y$. If $n \leq 2$, then any map $A \cup X^{(n)} \to \Sigma^{n-1}$ extends to all of X.*

2. *If $n \geq 3$, for any $x \in Z^{n-1}(X; \mathbb{Z})$ such that $x|_A = y$ we have that $x \smile_{n-3} x$ vanishes[3] on A, that is, it is element of $Z^{n+1}(X, A; \mathbb{Z}_2)$ (or element of $Z^4(X, A; \mathbb{Z})$ for $n = 3$) and it is a relative coboundary if and only if the corresponding map h can be extended to a map $X^{(n+1)} \to \Sigma^{n-1}$.*

We will use the notation $\Omega := \{x \in Z^{n-1}(X; \mathbb{Z})\colon x|_A = y\}$ further below. Test 1. above (corresponding to the primary obstruction) directly translates to an algorithm and the second one (the secondary obstruction) does so as well once $n > 3$. (We also explain what the notions of the primary and secondary obstructions mean exactly below.)

1. The set Ω corresponds to solutions of a linear equation over integers. To see that, let $\bar{y} \in C^{n-1}(X; \mathbb{Z})$ be an arbitrary cochain such that $\bar{y}|_A = y$. We have that

$$\Omega = \{\bar{y} - c\colon c \in C^{n-1}(X, A; \mathbb{Z}) \text{ such that } \delta c = \delta \bar{y}\}. \tag{3}$$

   Thus the extendability of f to $X^{(n)} \to \Sigma^{n-1}$ is equivalent to solvability of the linear equation $\delta c = \delta \bar{y}$ with the unknown $c \in C^{n-1}(X, A; \mathbb{Z})$.

2. Once Ω is nonempty, we fix $x \in \Omega$. From (3) it follows that there is a bijection $Z^{n-1}(X, A; \mathbb{Z}) \to \Omega$ given by $w \mapsto x - w$. Thus the extendability of f to a map $X^{(n+1)} \to \Sigma^{n-1}$ is equivalent to the existence of $w \in Z^{n-1}(X, A; \mathbb{Z})$ such that

$$\begin{aligned}&[(x-w) \smile_{n-3} (x-w)] = \\ &= [x \smile_{n-3} x] - [w \smile_{n-3} w] = \\ &= 0 \in H^{n+1}(X, A; \mathbb{Z}_2).\end{aligned}$$

We use that the map $w \mapsto w \smile_{n-3} w$ induces a homomorphism on the level of cohomology for $n > 3$, therefore the question reduces to a system of linear equations again. This formulation shows that the coset

$$[x \smile_{n-3} x] + \underbrace{Sq^2\big(H^{n-1}(X, A; \mathbb{Z})\big)}_{\{[w \smile_{n-3} w]\colon\, w \in Z^{n-1}(X,A;\mathbb{Z})\}}$$

of $H^{n+1}(X, A; \mathbb{Z}_2)$—called the *secondary obstruction*—captures the lack of extendability to the $(n+1)$st skeleton $X^{(n+1)}$. In the case $n = 3$ the extendability condition is $[(x - w) \smile (x - w)] = 0 \in H^4(X, A; \mathbb{Z})$ for some w which is computationally equivalent to solving systems of quadratic Diophantine equations—an undecidable problem [5]. In many instances, the quadratic equations are simple if not trivial and very simple heuristics suffice to solve them.

Robustness of the primary and secondary obstruction. In the persistent setting the input contains, in addition to above, a sequence of spaces $A_0 = A, A_1, \ldots, A_h$ and we want to compute a lower-bound on the robustness of non-extendability—a value k such that $f|_{A_k}$ cannot be extended to X for as large k as possible.

The key concept that allows an easy modification of the obstruction tests into the persistent setting is the functoriality of cohomology. For instance, the cochain extension $\bar{y}$ of $f^\sharp(z)$ is an extension of $f^\sharp|_{A_i}(z)$ for each $A_i \subseteq A$. The same holds for the cocycle extension x.

We state the algorithm **Primary–Secondary Persistence** for lower-bounding the robustness of non-extendability on a high-level fashion that emphasizes *what the algorithm does* rather that *how it is done*. The low level implementation is explained in the preprint [4].

0. Compute $y := f^\sharp(z) \in Z^{n-1}(A_0; \mathbb{Z})$. Fix an arbitrary extension $\bar{y} \in C^{n-1}(X; \mathbb{Z})$ of y.

1. Find the smallest $j \geq 0$ such that there is $c \in C^{n-1}(X, A_j; \mathbb{Z})$ such that $\delta c = \delta \bar{y}$. If $n = 1, 2$ output j. Otherwise let $x := \bar{y} - c$.

2. Find the smallest $k \geq j$ such that there is $b \in C^n(X, A_k; \mathbb{Z}_2)$ and $w \in Z^{n-1}(X, A_k; \mathbb{Z})$ such that $\delta b + w \smile_{n-3} w = x \smile_{n-3} x$. Output k.

Step 0 amounts to using the definition of the induced map in simplicial cohomology: namely, $f^\sharp(z)$ is defined to evaluate to 1 on the simplices $[v_1, \ldots, v_n]$ such that $[f(v_1), \ldots, f(v_n)] = [e_1, \ldots, e_n]$ and to evaluate to 0 once $\{f(v_1), \ldots, f(v_n)\} \neq \{e_1, \ldots, e_n\}$.

Step 1 and 2 are more involved and are reduced to matrix reductions over integers similar to those used in persistent homology computations over fields.

[3] By $x \smile_{n-3} x$ we denote a cocycle representant of the Steenrod square $Sq^2[x]$.

5 Experimental results with random fields.

One of our goals is to analyze how much "typical" is a situation in which the secondary obstruction or higher obstructions play a role. The lowest-dimensional case where nontrivial secondary obstruction can occur is $(m,n) = (4,3)$. We generated random continuous functions $f : [-1,1]^4 \to \mathbb{R}^3$ taken from different probability distributions and looked for possible nontrivial secondary obstructions. However, while the primary obstruction typically occurs whenever f contains a zero, we couldn't detect a single instance of a randomly generated function with nontrivial higher obstruction. Still, we don't dare to conclude that higher obstructions are untypical or unnatural, and think that more research is needed.[4] A short description of our first experiments follows.

First we considered random functions generated as Gaussian random fields. Each component $f_i(x)$ of $f(x)$ was generated so that for any finite set of points $\{x_1,\ldots,x_k\}$ the random vector $\{f_i(x_j) : j = 1,\ldots,k\}$ has a multivariate normal distribution with mean zero and the covariance between $f_i(x)$ and $f_i(y)$ was taken to be

$$C(x,y) = \exp(-\frac{|x-y|^2}{2l^2})$$

for suitable $l > 0$. We generated function values using $l = 1/2$, sampled from a grid $g^4 = 28^4 \subseteq [-1,1]^4$ with the three components of f generated independently.

For each trial, we first computed the minimal r_0 for which $f'|_{A^{\square}_{r_0}}$ is simplicial.[5] From a sample of 1218 functions, the average value of the minimal simplicial r_0 was 0.46. This value could be made smaller by refining the grid: however, in all cases, there was a nontrivial primary obstruction which persisted up to $r_1 > r_0$ whose value was in average 1.06. In all but three cases, there was no potential for a nontrivial secondary obstruction, because the cohomology group $H^4(X, A^{\square}_{r_1})$ was trivial. It was nontrivial in three cases, giving some hope for a nontrivial secondary obstruction, but there was no secondary obstruction in these cases either.[6]

One possible explanation for the lack of secondary obstruction is that the cohomology in dimension 4 has typically lower robustness than in dimension 3 and most generators have already died when the primary obstruction (element of H^3) dies. A similar phenomenon occurs in persistent homology of excursion sets of random scalar fields, where the persistence barcodes in dimension 0 die before the barcodes in dimension 1, compare [1]. The lack of top dimensional cohomology reflects the fact that most components of the zero set intersect the boundary of the domain: it will be a matter of future work to perform similar computations for functions defined on manifolds without boundary.

We also tried to detect higher obstructions in the vector fields $f(x) - f(0)$ where f was generated as above and 0 is the midpoint of the $[-1,1]^4$ cube, with the hope of isolating the zero set farther from the boundary. The top cohomology was indeed richer, but no secondary obstruction was detected either. We also tried to use other covariance functions but the results were similar.

Our last attempt to detect secondary obstruction in random fields was to generate random homogenous quadratic polynomials. The coefficients a^k_{ij} in $f_k(x) = \sum_{i,j} a^k_{i,j} x_i x_j$ were generated as independent samples from a standard normal distribution.[7] The zero set of homogenous quadratic functions is either the origin alone or a cone intersecting the boundary $\partial[-1,1]^4$: only the first case can yield a nontrivial $H^4(X, A^{\square}_r)$ and a nontrivial secondary obstruction. We generated around 70 thousand instances of random quadratic functions on a 10^4 grid: around 2.2% of them had only the origin as the zero set, but there was no nontrivial secondary obstruction in a single instance.

[4] While we were not able to detect higher obstructions in random fields, they occur in relatively simple examples with component-wise quadratic functions.

[5] In our implementation, we work with a triangulation $A^{\square}_r$ of the cubical complex that consists of all cubes c such that $|f(x)| \geq r$ for all vertices of c, rather than with A_r defined above.

[6] We assume that in these three cases, nontriviality of $H^4(X, A^{\square}_r)$ was induced by a local positive minimum of $|f|$ in the interior of the domain, rather then by a neighborhood of zero set.

[7] This is motivated by the fact that simplest examples of functions with nontrivial secondary obstruction are quadratic and homogenous.

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