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Invariance and convergence of partitioning based optimisation algorithms in non-linear, non-continuous search spaces

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Abstract The class of optimisation problems studied here are general non-linear programming (NLP) problems with non-smooth, non-continuous objective and constraint functions. These problems fall within the category of constrained derivative free optimisation (DFO), although results also hold for discrete optimisation problems such as mixed integer non-linear programming (MINLP). Lipschitzian-based partitioning techniques are commonly employed by global optimisation algorithms to find solutions to DFO problems that are assumed to be Lipschitz smooth; here some of their properties are extended to the case where the functions cannot be assumed to be Lipschitz smooth. The concept of invariance as used in the context of algebraic topology is connected rigorously to the concept of convergence to a global minimum as used in the context of global optimisation and NLP through a simplicial homology. It is proved that all spatial partitioning algorithms with triangulable partitioning spaces will converge to the global optimum in finite time when provided with simple additional constructions. Particular emphasis is placed on analysis of the simplicial homology global optimisation (SHGO) algorithm; a general purpose global optimisation algorithm based on applications of simplicial integral homology and combinatorial topology. The homology built on an objective function presents a new way of visualising the multimodality of problems in hyperspace. This allows for rigorous performance investigation of algorithms relying on everywhere dense sampling sets in global convergence proofs.

Keywords Global optimisation · Derivative free optimisation · SHGO · Computational homology

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1 Introduction

In this publication we develop novel properties for a number of constrained derivative free optimisation (DFO) algorithms. In particular these include a family of algorithms classified as Lipschitzian-based partitioning techniques by **?**] which include the algorithm developed by **?**], DIvide a hyper- RECTangle (DIRECT) [**?**] and Branch-and-bound (BB) algorithms. However, similar constructions are possible for any algorithm using a response surface or covering space that fully covers the search space and is triangulable. For example the hypercube is triangulable [**?**], therefore the family of DIRECT algorithms based on [**?**] will inherit these properties. It is further proved that any topological properties that are proven to hold within a compact domain space, also hold across non-compact domain spaces after adequate refinement as defined through the proof.

Mainly it is shown how homological invariance can be used as a gateway to proving convergence across disconnected, well behaved sub-domains on non-continuous objective functions. Most of these algorithms were inherently designed for Lipschitz smooth objective functions. However, we will show that very simple additional constructions can guarantee global convergence on a broader class of problems. The full abstract constructions used in the proofs are employed in the simplicial homology global optimisation (shgo) algorithm [**? ?**], but the properties are inherent in the modified objective function defined in Definition 11, therefore only this modification is required (implemented in practice by using a simple wrapper) to retain global convergence guarantees. An explicit triangulation is unnecessary; the spacial partitioning need only be known to be triangulable.

In the most general case of the DFO optimisation problems discussed here are of the form:

$$\begin{aligned} \inf_{x} \quad & f(\mathbf{x}),\ \mathbf{x} \in \mathbb{R}^n \\ \text{s.t.} \quad & g_i(\mathbf{x}) \geq 0,\ \forall i = 1, ..., m \\ & h_j(\mathbf{x}) = 0,\ \forall j = 1, ..., p \end{aligned} \tag{1}$$

- $\mathbf{x}$ is a vector of one or more variables.
- $f(\mathbf{x})$ is the objective function $f : \mathbb{R}^n \to \mathbb{R}$.
- $g_i(\mathbf{x})$ are the inequality constraints $\boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^m$.
- $h_j(\mathbf{x})$ are the equality constraints $\boldsymbol{h} : \mathbb{R}^n \to \mathbb{R}^p$.

The real objective function $f(\mathbf{x})$ maps a vector of dimension n to a scalar value. It is important to note that $\mathbb{R}$ is the codomain of f, but the image of f is inherently unknown (a subset of $\mathbb{R}$). It can be either smooth or non-smooth. In the most general case f is a non-convex, non-continuous function. In this publication we will describe the concept of sub-domains wherein f behaves as a Lipschitz continuous function which should be clear from the context. In addition it is assumed that the objective function has a finite number of local minima. Note that a local minimum does not always exist[1]. So we are in fact looking for a local infimum of the feasible search space. Finally, the variables $\mathbf{x}$ are assumed to be bounded. For example if lower and

[1] for example consider the piece-wise linear function $f = x + 1\ \forall x \geq 0$, and $-x\ \forall x < 0$

upper bounds l_i and u_i are implemented for each variable then we have an initially defined hyperrectangle

$$z\mathbf{x} \in \Omega \subseteq [\mathbf{l}, \mathbf{u}]^n \;=\; [l_1,\; u_1] \;\times\; [l_2,\; u_2] \;\times\; \ldots \;\times\; [l_n,\; u_n] \subseteq \mathbb{R}^n \tag{2}$$

where Ω is the limited feasible subset excluding points outside the bounds and constraints.

$$\Omega = \{\mathbf{x} \in [\mathbf{l}, \mathbf{u}]^n \mid \mathbf{g}_i(\mathbf{x}) \geq 0 \, \forall i \in \mathbb{Z}_m, h_j(x) = 0 \, \forall j \in \mathbb{Z}_j\} \tag{3}$$

For example when the constraints in $\mathbf{g}$ are linear and there are no equality constraints then the set Ω is always a compact space.

The convergence of the DIRECT [**? ?**] algorithm in non-compact spaces (caused for example by general, non-linear inequality constraint) was previously proven by **?**], however, in [**?**] it is required that f be Lipschitz continuous in the domain $[\mathbf{l}, \mathbf{u}]^n$. In [**? ?**] the objective function is modified by what is referred to as "hidden constraints" which are detected when f fails to return a value. We will show that this is an equivalent construction to the one described in this publication and therefore the condition of Lipschitz continuity is unnecessary since the software implementation of [**?**] will converge to the global minimum under the larger class of problems described in Equation 1. Many algorithms in literature are derived from DIRECT. For example the novel DISIMPL (DIviding SIMPLices algorithm [**? ? ?**] is based on DIRECT and is also proven to converge in compact spaces while showing much greater performance than DIRECT under certain conditions such as problems with linear constraints.

In building towards the proof we start by rigorously defining a simplicial complex approximation of the objective function f. Several theorems applying to compact Lipschitz spaces were proven in [**?**] which will be reviewed and used to prove an invariance across discontinuous spaces (a homology on f). Finally it is shown that convergence follows trivially from the invariance.

2 Directed simplicial complex approximation of the objective function

Consider the general objective function mapping in real space $f : \mathbb{R}^n \to \mathbb{R}$. The purpose of this section is to describe a discrete mapping $h : \mathcal{P} \to \mathcal{H}$ to provide a simplicial approximation for the surface of f. Describing this construction will require several concepts from algebraic and combinatorial topology [**?**]. The following definition was adapted from **?** , p. 9]

Definition 1 A ***n*-simplex** is a set of $n+1$ vertices in a convex polytope of dimension n. Formally if the $n+1$ points are the $n+1$ standard $n+1$ basis vectors for $\mathbb{R}^{(n+1)}$. Then the n-dimensional n-simplex is the set

$$S^n = \left\{ (t_1, \ldots, t_{n+1}) \in \mathbb{R}^{n+1} \mid \sum_1^{n+1} t_{n+1} = 1, t_i \geq 0 \right\}$$

For example, a 2-simplex is a triangle and a 3-simplex is a tetrahedron. We will use the following combinatorial definition of a simplicial complex [**?** , p. 107]

Definition 2 A **simplicial complex** $\mathcal{H}$ is a set $\mathcal{H}^0$ of vertices together with sets $\mathcal{H}^n$ of n-simplices, which are $(n+1)$-element subsets of $\mathcal{H}^0$. The only requirement is that each $(k+1)$-elements subset of the vertices of an n-simplex in $\mathcal{H}^n$ is a k-simplex, in $\mathcal{H}^k$.

Thus each n-simplex has $n+1$ distinct vertices, and no other n-simplex has this same set of vertices.

In this publication the $\mathcal{H}$ symbol will be used to represent a (finite) simplicial complex rather than the more standard Δ to avoid confusion with the difference and Laplacian operators common in optimisation. The superscript $\mathcal{H}^k$ represents the subset of $k-$dimensional simplices where for an n dimensional problem the highest dimensional $k-$simplex contains $n+1$ vertices. Finally we define a k-chain [**?**]

Definition 3 A **k-chain** is a union of simplices.

For example a 0-chain is a set of vertices, a 1-chain is a set of edges and a 2-chain is a set of triangles. $C(\mathcal{H}^k)$ denotes a $k-$chain of $k-$simplices. A vertex in $\mathcal{H}^0$ is denoted by v_i. If v_i and v_j are two endpoints of a directed edge in $\mathcal{H}^1$ from v_i to v_j then the symbol $\overline{v_i v_j}$ represents the edge so that it is bounded by the $0-$chain $\partial\left(\overline{v_i v_j}\right) = v_j - v_i$ and similarly for an edge directed from v_j to v_i, we have, $\partial\left(\overline{v_j v_i}\right) = \partial\left(-\overline{v_i v_j}\right) = v_i - v_j$. Higher dimensional simplices can be represented and directed in a similar manner, for example a triangle consisting of three vertices v_i, v_j and v_k directed as $\overline{v_i v_j v_k}$ has the boundary of directed edges $\partial\left(\overline{v_i v_j v_j}\right) = \overline{v_i v_j} + \overline{v_j v_k} + \overline{v_j v_i}$.

We start by formally defining the set of vertices from which 0-chains of the simplicial complex $\mathcal{H}$ are built and the edges from which the 1-chains of $\mathcal{H}$ are built.

Definition 4 Let $\mathcal{X}$ be the set of sampling points generated by a sampling sequence in the bounded hyperrectangle $[\mathbf{l}, \mathbf{u}]^n$. The set $\mathcal{P} = \{\mathbf{x} \in \mathcal{X} \mid \mathbf{g}(\mathbf{x}) \geq 0\}$ is a set of points within the feasible set Ω .

Definition 5 For an objective function f, $\mathcal{F}$ is the set of scalar outputs mapped by the objective function $f : \mathcal{P} \to \mathcal{F}$ for a given sampling set $\mathcal{P} \subseteq \Omega \subseteq \mathbb{R}^n$.

Definition 6 Let $\mathcal{H}$ be a directed simplicial complex. Then $\mathcal{H}^0 := \mathcal{P}$ is the set of all vertices of $\mathcal{H}$.

Definition 7 For a given set of vertices $\mathcal{H}^0$, the simplicial complex $\mathcal{H}$ is constructed by a triangulation connecting every vertex in $\mathcal{H}^0$. The triangulation supplies a set of undirected edges E.

Definition 8 The set $\mathcal{H}^1$ is constructed by directing every edge in E. A vertex $v_i \in \mathcal{H}^0$ is connected to another vertex v_j by an edge contained in E. The edge is directed as $\overline{v_i v_j}$ from v_i to v_j iff $f(v_i) < f(v_j)$ so that $\partial\left(\overline{v_i v_j}\right) = v_j - v_i$. Similarly an edge is directed as $\overline{v_j v_i}$ from v_j to v_i iff $f(v_i) > f(v_j)$ so that $\partial\left(\overline{v_j v_i}\right) = v_i - v_j$.

For practical computational reasons we must also consider the case where $f(v_i) = f(v_j)$. If neither v_i or v_j is already a minimiser (see Definition 9) we will make use of rule that the incidence direction of the connecting edge is always directed towards the vertex that was generated earliest by the sampling point sequence. If v_i is not connected to another vertex v_k then we leave the notation $\overline{v_i v_k}$ undefined and let $\partial\left(\overline{v_i v_k}\right) = 0$. We let the higher dimensional simplices of $\mathcal{H}^k, k = 2, 3, \ldots n+1$ be directed in an arbitrary direction which completes the construction of the complex $h : \mathcal{P} \to \mathcal{H}$. We can now use $\mathcal{H}$ to find the minimiser pool for the local minimisation starting points used by the algorithm:

Definition 9 A vertex v_i is a minimiser iff every edge connected to v_i is directed away from v_i, that is $\partial\left(\overline{v_i v_j}\right) = (v_{j\neq i} - v_i) \vee 0 \, \forall v_{j\neq i} \in \mathcal{H}^0$. The minimiser pool $\mathcal{M}$ is the set of all minimisers.

3 Locally convex sub-domains and invariance of the directed complex within a bounded hyperrectangle

3.1 Sub-domains of Ω

Consider a rectangular sub-domain $\Psi \subseteq \Omega$ with the exact geometric shape of $[\mathbf{l}, \mathbf{u}]^n$ wherein f is Lipschitz smooth. In Section 4 we will demonstrate that these subdomains can be found, if they exist, in any space Ω, but in this section it is important to consider Ψ independently of Ω in order to build and understand the topological properties of Ψ. Such a space is compact, Theorem 1 was previously proved by **?**]:

Theorem 1 *Given a minimiser $v_i \in \mathcal{M} \subseteq \mathcal{H}^0$ on the surface of a continuous, Lipschitz smooth objective function f with a compact bounded domain in $\mathbb{R}^n$ and range $\mathbb{R}$, there exists at least one stationary point of f within the domain defined by st (v_i).*

Theorem 1 is built on previous results of Brouwer's fixed point theorem [**?**] found in for example **?** , p. 40] utilising Sperner's lemma. It is essentially an generalisation of the combinatorial version of the classical fixed point theorem and can be used to find proven local minima together with their compact, locally convex sub-domains (st (v_i)) in spaces that allow for general constraints (analogous to the Karush–Kuhn–Tucker (KKT) generalisation of the method of Lagrange multipliers). In addition the extension allows for the detection of one or more sub-domains with proven fixed points on the gradient vector fields of black-box numerical functions. Note that finding st $(v_i) \subset \Psi \subseteq \Omega$ relies on the refinement of $\mathcal{H}$ through h by using increased sampling $\mathcal{P}$. This theorem applies to any subdomain Ψ. The usefulness of Theorem 1 is immediately obvious (a starting point in a well defined attractor with added constraints in ∂ (st (v_i)) can quickly find the local infimum). However, it is even more important as geometric marker from which we may induce topological properties of our problem (a homology built on f). To understand how this homology relates to other computational homologies it is useful to imagine the inverse of a bounded gradient field which has singularities at local minima.

Theorem 1 is built on Sperner's lemma.

Theorem 2 *(Sperner's lemma [**?**]) Every Sperner labelling of a triangulation of a n-dimensional simplex contains a cell labelled with a complete set of labels: 1,2, . . . , n+1.*

The abstractions allows for many useful results from the field of algebraic topology. For example **?**] where they proved the Atanassov conjecture [**?**] that for any polytope with N vertices there are $N - n$ simplices that receive a complete set of Sperner labels. **?**] further extended this theorem and more recently **?**] extended the theorems to a large class of manifolds with or without boundary.

The theorems by Meunier and Musin allow us to extend Sperner's lemma to a simplicial complex built in a $(n + 1)$-dimensional non-euclidean space. This would allow the application of ideas from discrete differential geometry. For example the Gauss-Bonnet theorem holds for discrete simplicial surfaces [**?**].

In global optimisation theory a simplicial complex built in this space can be used for approximating local and global Lipschitz constants for an objective function while still retaining the ability to detect locally convex sub-domains in the search space. Furthermore it allows for any results of optimisation problems in real euclidean spaces to be used in a large class of other spaces.

3.2 Invariance of $\Psi \subseteq \Omega$

For black box functions there is no way to know if the number and distribution of sampling points is adequate without more information (for example if the number of local minima are known in the problem). However, it is an important property of the algorithm that $|\mathcal{M}|$ will stop increasing with higher sampling after this point. First we define an adequately sampled surface.

Definition 10 Consider a simplicial complex $\mathcal{H}$ built on an objective function f with a compact feasible set Ψ using Definitions 6 through 9. The surface is said to be **adequately sampled** if there is one and only one true stationary point within every domain defined by Theorem 1.

Finally we state following theorem proved in [**?**] which holds in the case where $\Psi = [\mathbf{l}, \mathbf{u}]^n$.

Theorem 3 *(Invariance of an adequately sampled simplicial complex $\mathcal{H}$) For a given continuous objective function f that is adequately sampled by a sampling set of size N. If the cardinality of the minimiser pool extracted from the directed simplex $\mathcal{H}$ is $|\mathcal{M}|$. Then any further increase of the sampling set N will not increase $|\mathcal{M}|$.*

The proof provided in [**?**] relies on a homomorphism between the simplicial complex $\mathcal{H}$ constructed in the bounded hyperrectangle Ψ and the homology (mod 2) groups of a constructed surface $\mathcal{S}$ on which we can invoke the Invariance theorem as defined in fundamental homologies such as **?**]. We review some of the abstract geometric and topological mechanisms used in this proof, which will aid in understanding the proof in Section 4.

?] defined the n-torus $\mathcal{S}_0$ from the compact, bounded hyperrectangle Ψ by identification of the opposite faces and all extreme vertices. Now for every strict local minimum point $\mathbf{p} \in \Psi$ puncture a hypersphere and after appropriate identification the resulting n-dimensional manifold $\mathcal{S}_g$ is a connected g sum of g tori $S := S_0 \# S_1 \# \cdots \# S_{g-1} \qquad (g \text{ times})$.

Figures 1 and 2 demonstrate the process geometrically. Figure 1 shows how to puncture a hypersphere and make the usual identifications in a 2-dimensional problem. Figure 2 demonstrates the construction of $\mathcal{S}_g$.

4 Invariance and convergence of non-continuous, non-linear optimisation problems with bounded variables

In this section we present the main contribution of this paper. Consider again Equation 1, but now we are working with the fully general case where $\mathbf{g}$ is non-linear and Ω is not a compact set. In addition we allow f to be non-continuous (in having removable or jump discontinuities across large sub-domains) and non-linear. It is still assumed that the variables $\mathbf{x}$ are bounded. Furthermore we assume that there is a feasible solution so that $\Omega \neq \emptyset$ and that there exists at least one point in the range of f mapped within the domain Ω. We will prove that if the simplicial sampling sequence[2] [**?**] is used, then SHGO will retain the invariance property of Theorem 3. Secondly convergence of the SHGO algorithm is proved when the number of sampling points tends to infinity.

Before proving these properties we will need to define a new construction to deal with discontinuities in f. From Definition 4 and Definition 5 it is clear that f will only map a subset of feasible domain Ω, therefore only points within the this domain need to be considered. A new construction replacing Definition 5 that considers discontinuities (such as singularities) in the hypersurface of f is now defined:

Definition 11 For an objective function f, $\mathcal{F}$ is the set of scalar outputs mapped by the objective function $f : \mathcal{P} \to \mathcal{F}$ for a given sampling set $\mathcal{P} \subseteq \Omega \subseteq \mathbb{R}^n$. If a mapping of a vertex v_i does not exist, then we define the mapping as $f : v_i \to \infty$. Any such point is excluded from the set $\mathcal{M}$.

Note from Definition 8 that any vertex v, $f(v) = \infty$ that is connected to another vertex in Ω that maps to a finite value will never be a minimiser. This simple construction allows us to develop the following theorem:

Theorem 4 *(Invariance of an adequately sampled simplicial complex $\mathcal{H}$ in a non-convex, non-compact space Ω). For a given non-continuous, non-linear objective function f that is adequately sampled by a sampling set of size N. If the cardinality of the minimiser pool extracted from the directed simplex $\mathcal{H}$ is $|\mathcal{M}|$. Then any further increase of the sampling set N will not increase $|\mathcal{M}|$.*

Proof Theorem 3 holds for any compact hyperrectangular space $\mathbb{B}_0 = [x_l^1, x_u^1] \times [x_l^2, x_u^2] \times \cdots \times [x_l^n, x_u^n]$. Consider a set of subspaces $\mathbb{B}_i \cong \mathbb{B}_0$ with $\mathbb{B}_i \subseteq \Omega \; \forall i \in \mathbf{I}$. That is, $\mathbb{B}_i$ is any compact, rectangular subspace of Ω that is homeomorphic to $\mathbb{B}_0$ (which is also homeomorphic to a point) and can, therefore, be shrunk or expanded to arbitrary sizes while retaining compactness. Therefore any triangulation $\mathcal{K}_i$ of $\mathbb{B}_i$ retains the invariance property from Theorem 3.

[2] This sampling sequence refines a simplicial complex by sub-dividing the largest face of its simplices and has the property that after every iteration the subdivisions of the complex are symmetric and isomorphic to the initial triangulation

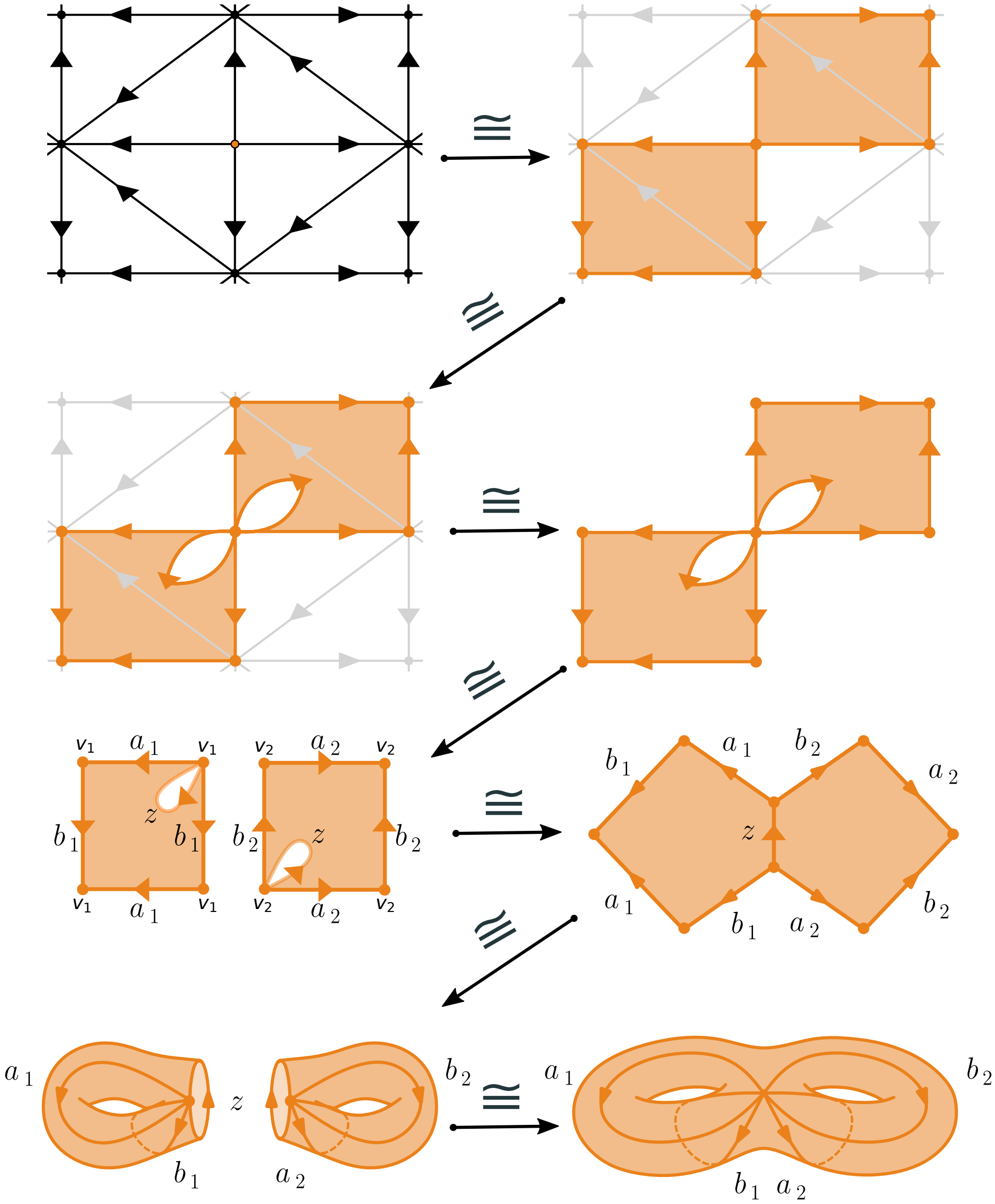

Fig. 1 The process of puncturing a hypersphere at a minimiser point in a compact search space. Start by identifying a minimiser point in the $\mathcal{H}^1$ ($\cong$ $\mathcal{K}^1$) graph. By construction, our initial complex exists on the (hyper-)surface of an n-dimensional torus $\mathcal{S}_0$ such that the rest of $\mathcal{K}^1$ is connected and compact. We puncture a hypersphere at the minimiser point and identify the resulting edges (or $(n-1)$-simplices in higher dimensional problems). Next we shrink (*a topological (ie continuous) transformation*) the remainder of the simplicial complex to the faces and vertices of our (hyper-)plane model. Make the appropriate identifications for $\mathcal{S}_0$ and glue the identified and connected face z (a $(n-1)$-simplex) that resulted from the hypersphere puncture. The other faces (ie $(n-1)$-simplices) are connected in the usual way for tori constructions)

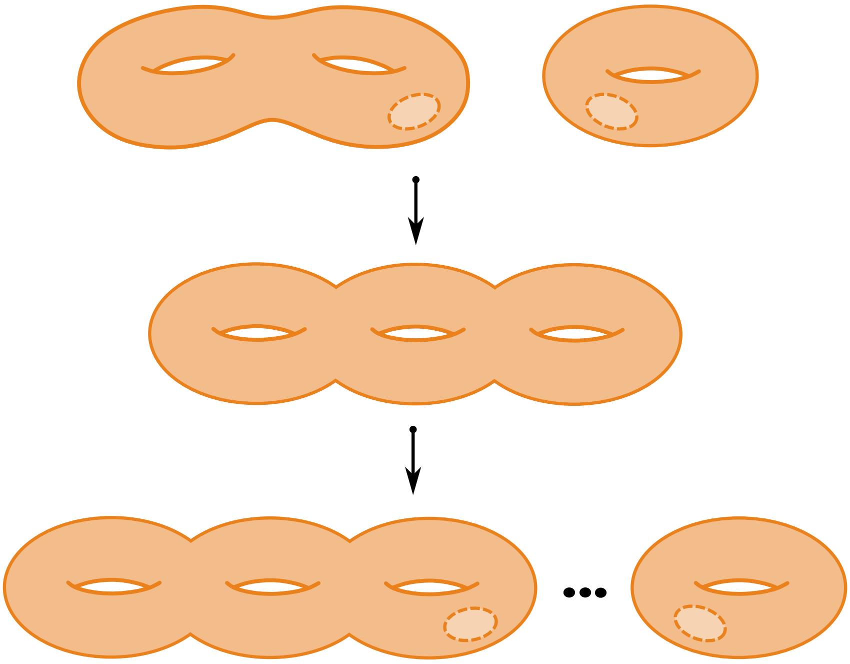

Fig. 2 The process of puncturing a new hypersphere on $\mathcal{S}_0 \# \mathcal{S}_1$ can be repeated for any new minimiser point without loss of generality producing $S := S_0 \# S_1 \# \cdots \# S_{g-1} \qquad (g \text{ times})$

We allow all $\mathbb{B}_i$ to be connected or disconnected subspaces with respect to any other $\mathbb{B}_{j \in I}$ within Ω. Now consider the (mod 2) homology groups $\mathbf{H}_1(\mathcal{K}_i)$ of $\mathcal{K}_i$. Since the homology groups are abelian groups the rank is additive over arbitrary direct sums:

$$\operatorname{rank}\left(\bigoplus_{i \in I} \mathbf{H}_1(\mathcal{K}_i)\right) = \sum_{i \in I} \operatorname{rank}(\mathbf{H}_1(\mathcal{K}_i))$$

Therefore the triangulations of both connected and disconnected subspaces $\mathbb{B}_i$ within a possibly non-compact space Ω will retain the same total rank. After adequate sampling, the rank of $\mathbf{H}_1(\mathcal{K}_i)$ will not increase by Theorem 3. Any point that is not in Ω is not connected to any graph structure by Definition 4 and Definition 5 and therefore cannot increase the rank of any homology group $\mathbf{H}_1(\mathcal{K}_i)$. Finally any vertex $v_i \in \Omega$ for which $f(v_i)$ does not exist will by Definition 11 be mapped to infinity by Definition 11. By Definition 9, v_i can not be a minimiser and therefore cannot increase the rank of any homology group $\mathbf{H}_1(\mathcal{K}_i)$. Figure 3 demonstrates this property geometrically.

We have shown that the total rank of the homology groups triangulated on all connected and disconnected subspaces $\mathbb{B}_i \in \Omega$ will not increase after adequate sampling. It remains to be proven that these subspaces exist within Ω. We adapt the proposition used in the convergence proof by **?**] for subdivided simplicial complexes.

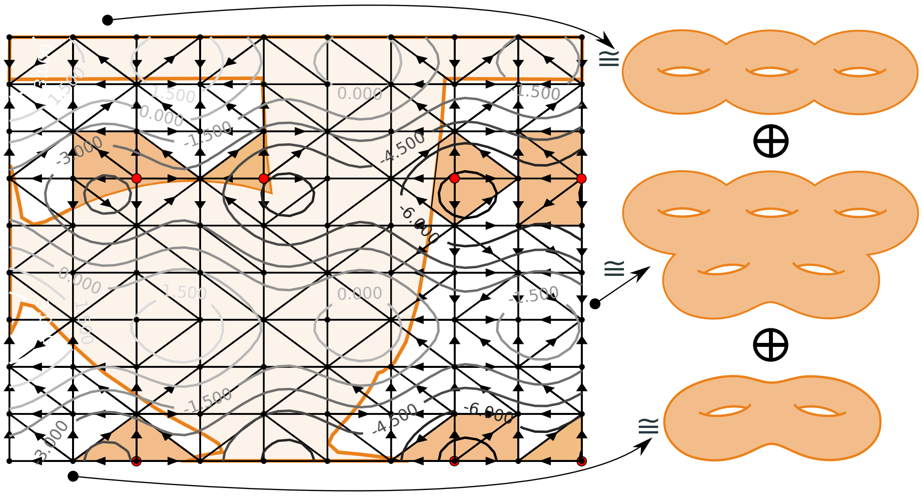

Fig. 3 Visual demonstration on surfaces with non-linear constraints, the shaded region is unfeasible. The vertices of the points mapped to infinity have undirected edges, therefore they do not form simplicial complexes in the integral homology. The surfaces of each disconnected simplicial complex $\mathcal{K}_i$ can be constructed from the compact version of the invariance theorem. The rank of the abelian homology groups $\mathbf{H}_1(\mathcal{K}_i)$ is additive over arbitrary direct sums

Proposition 1 *For any point* $\mathbf{x} \in \Omega$ *and any* $\epsilon > 0$ *there exists an iteration* $k(\epsilon) \geq 1$ *and a point* $\mathbf{x}_i^k \in \mathcal{H}^n \in \Omega$ *such that* $\left\|\mathbf{x}_i^k - \mathbf{x}\right\| < \epsilon$*.*

Sampling points $\mathbf{x}_i$ are vertices $\mathcal{H}^0$ belonging to the set of n-dimensional simplices $\mathcal{H}^n$. Let δ_{max}^k be the largest diameter of the largest simplex. Since the subdivision is symmetrical all simplices have the same diameter δ_{max}^k after every iteration of the complex. At every iteration the diameter will be divided through the longest edge, thus reducing the simplices' volumes. After a sufficiently large number of iterations all simplices will have the diameter smaller than ϵ. Therefore the vertices of the complex will converge to any and all points inside compact subspaces $\mathbb{B}_i$ within Ω. Since we have assumed that $\Omega \neq \emptyset$ this proves the existence of subspaces $\mathbb{B}_i$.

This concludes the proof of Theorem 4

From this proof the convergence to a global minimum within Ω, if it exists, also trivially follows by noting that $\mathbb{B}_i$ is homeomorphic to a point and that Theorem 1 applies to any minimiser in $\mathbb{B}_i$. In practice Definition 11 is implemented in **?**] by using exception handling that can capture any mathematical errors in addition to converting any non-float objects/numbers outputted by an objective function to infinite floating point values that are defined to be greater than any other floating point values.

5 Numerical example: the geometry and topology of non-continuous global optimisation

5.1 Optimisation across discontinuities in f

This section demonstrates the principles behind the proof of Theorem 4 using a numerical example that is easy to visualise rather than assessing any performance on functions with Lipschitz discontinuities which is beyond the scope of this paper. Consider the following numerical example which contains a number of different types of discontinuities.

Example 1 Consider an optimisation instance defined by the following objective function together with its domain $\Omega \subseteq [-\mathbf{4.5}, \mathbf{4.5}]^n$

$$f(\mathbf{x}) = \begin{cases} \sqrt{x_1^2 - 3} + \sum_{i=1}^{2}(x_i^2 + 5x_i) + 25\left(\sin^2(x_1) + \cos^2(x_2)\right) & \forall x_1 \geq -1 \\ \sqrt{x_1^2 - 3} + \sum_{i=1}^{2}(x_i^2 + 5x_i) + 25\left(\sin^2(x_1) + \cos^2(x_2)\right) + 50 & \forall x_1 < -1 \end{cases} \tag{4}$$

A 3-dimensional plot is provided in Figure 4. There are six local minima and one global minimum. Note that negative square roots are not defined in real space, the large discontinuities are representative of the mathematical and numerical errors encountered when computing objective functions. In Figure 5 we show the directed simplicial complex approximation of f and their homology constructs. It is observed that the algorithm initially assumes that Ω is compact, however, subsequent refinement demonstrates discontinuities and the disconnected subgraphs search for compact sub-domains. In Figure 6 we demonstrate that further refinement does not alter the homology group rank of the simplicial complex. Figure 6 further demonstrates how the star domain sub-spaces of $\mathrm{st}(v)$ are refined to locally convex sub-domains of Ω.

5.2 Performance discussion

The reliance on everywhere dense sets for convergence is questionable with respect to the performance of algorithms. For example **?**] showed that in some cases algorithms must essentially reduce to a brute force. In general efficient global optimisation requires global information. However, in many black-box problems global information is difficult or impossible to obtain. For example it is obviously the case that discontinuous functions do not have global Lipschitz bounds.

The rigorous concept of adequate sampling proves both that the shgo algorithm finds the global minimum before sets are everywhere dense (unless the solution space is also everywhere dense) and that sub-domains can be used to obtain approximate global properties of f in the form of an invariance on f. For example Figure 7 demonstrates the homology group growth on Example 1 as the number of sampling points is increased. This tool can be used by an optimisation practitioner to aid in the visualisation of the behaviour of a function f which can't be visualised in hyperspaces of arbitrary dimensions (by for example plotting the surface). Informally, the growth

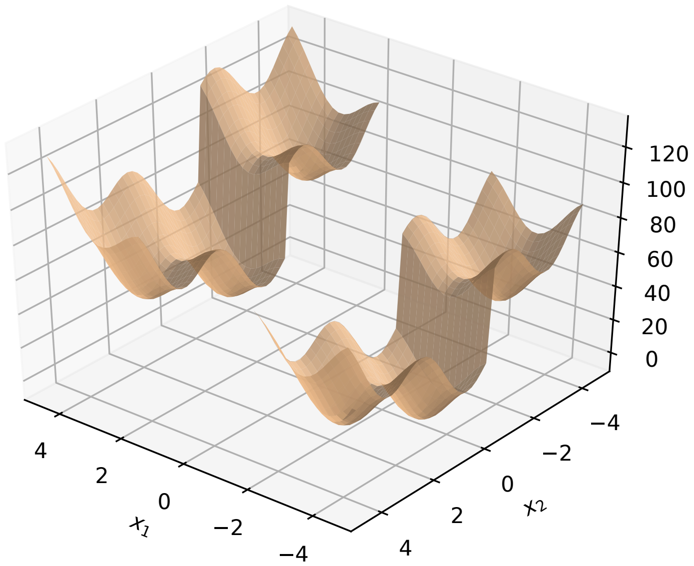

Fig. 4 3-dimensional surface plot of Example 1

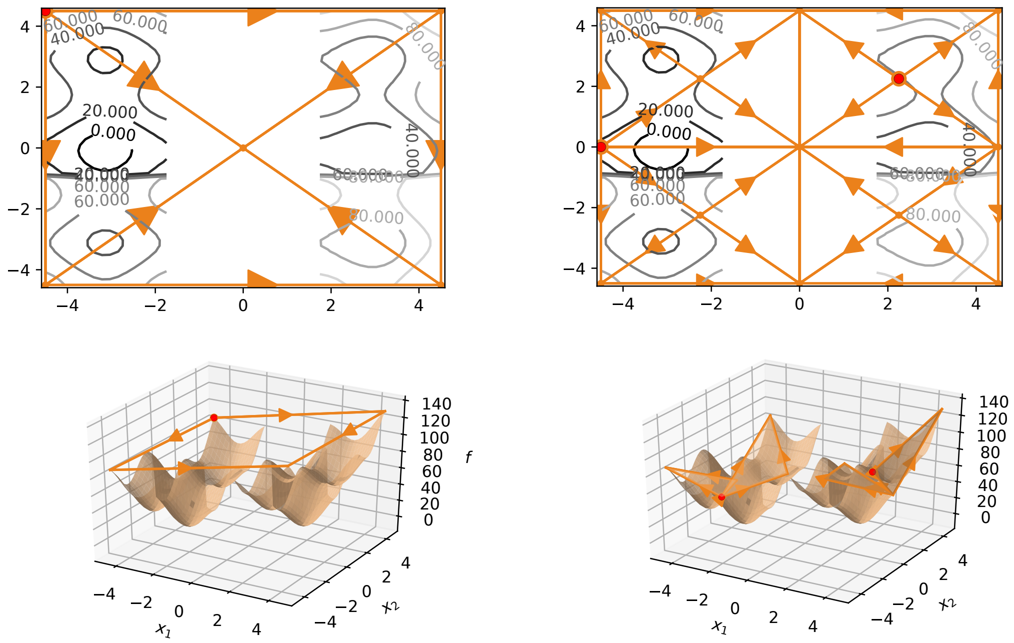

Fig. 5 Refinements into disconnected sub-graphs of Example 1 across its discontinuities. The contour and surface plots of the objective function and a simplcial complex appromixation after an initial triangluation given is shown on the left and a first iteration of initial refinement is shown on the right. The larger, red vertices are minimiser points

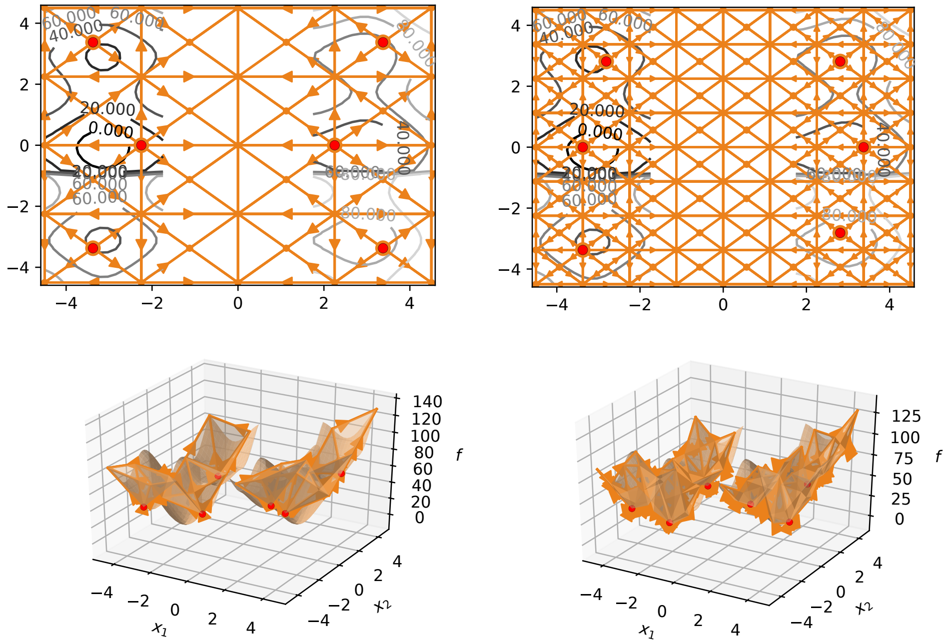

Fig. 6 Further refinement does not increase the homology group ranks of $\mathcal{H}$

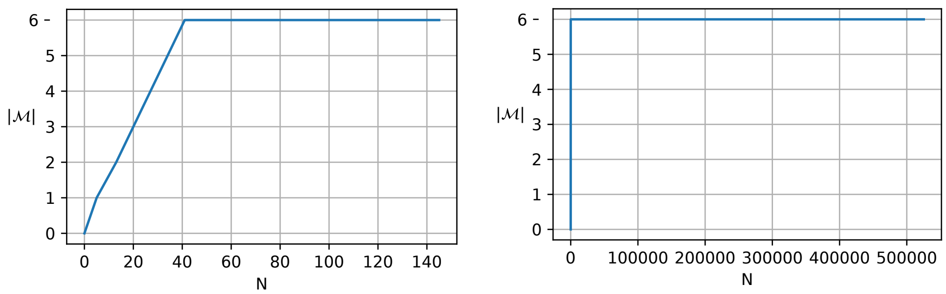

Fig. 7 Homology group growth of Example 1 across its discontinuities as a function of sampling points N

rate of the homology group rank of $\mathbf{H}_1(\mathcal{H}_1)$ is a measure of the approximate sparsity of solutions and the pathology of f. The approximate equilibrium value of the rank of $\mathbf{H}_1(\mathcal{H}_1)$ as N becomes arbitrarily large (the growth is not always monotone) is a measure of the multi-modality of f.

We note at this point that the inverse of Theorem 4 is not true. In other words a stop in $|\mathcal{M}|$ growth over iterations does not imply that the search space has been adequately sampled. These figures demonstrate the theoretical convergence of an algorithm using topological deductions. Therefore in practice $|\mathcal{M}|$ is mostly useful as a heuristic, but cannot be used as a rigorous stopping criteria unless $|\mathcal{M}|$ is known *a-priori*.

5.3 Singularities in f

The minimization of a function with infinite discontinuities on f has not been well defined on Equation 1. Infinite discontinuities where the objective function becomes arbitrarily large $f \to +\infty$ at a vector $\mathbf{x}_\infty$ are simple enough to understand and fit in well with our restructured objective function Definition 11. These points largely behave largely the same as any other points in unfeasible domains. However, when the objective function becomes arbitrarily small at $\mathbf{x}_\infty$, $f \to -\infty$, the solution to Equation 1 becomes more difficult to define. For example the point $\mathbf{x}_\infty$ is smaller than any point in Ω, however, since the limit of the objective function is not defined at $\mathbf{x}_\infty$, it is not the infimum of Ω. A precise rigorous definition is a subject of real analysis and will not be discussed in depth in this publication. However, in optimisation practice the solution to Equation 1is defined within some percentage error. Therefore any point $\mathbf{x}^*$ near the infinite discontinuity $\mathbf{x}_\infty \leftarrow \mathbf{x}^*$ within some tolerance of $\left\|\mathbf{x}_i^k - \mathbf{x}\right\| < \epsilon$ is considered a solution to Equation 1. In this neighbourhood the usual notion of compact sub-domains still apply, the algorithms will seek well behaved sub-domains that a contain a point $\mathbf{x}^* \leftarrow \mathbf{x}_\infty$. In addition there is an arbitrarily small sub-domain bounded by $\partial\left(\mathrm{st}\left(\mathbf{x}^*\right)\right)$ that is well behaved. As discussed in this section finding this solution on a pathological surface reduces to brute force.

6 Conclusion

By constructing a homology on the objective function f we have shown that the convergence of spatial partitioning algorithms to the global minimum trivially follows from the invariance of the homology. Furthermore we have shown that computing and tracking the homology groups on f connects the concept of well-behaved functions to a compatible metric that can be defined on objective functions of arbitrary finite dimensions.

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