Simplicial Homology Global Optimisation

A Lipschitz global optimisation algorithm

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https://stefan-endres.github.io/shgo/files/shgo_slides.pdf ▸ Link

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Introduction

Introduction

- Global optimisation of black-box functions
- Simplicial complexes built from sampling points
- Use simplicial complexes to extract information about the objective function (hyper-)surface using:
  - Simplicial integral homology theory
  - Discrete exterior calculus
  - Combinatorial and algebraic topology
- Information extracted in the limits:
  - Number of locally convex sub-domains (a measure of multi-modality)
  - Points in neighbourhoods of local minima
  - Locally convex sub-domains around (with explicit constraints defining these domains)
- The full simplicial homology global optimisation (shgo) algorithm passes the extracted starting points from the global search to find the local minima including global minimum

Properties

Properties of shgo:

- Convergence to a global minimum assured for Lipschitz smooth functions
- Allows for non-linear constraints
- Extracts all the minima in the limit of an adequately sampled search space (assuming a finite number of local minima)
- Progress can be tracked after every iteration through the calculated homology groups
- Competitive performance compared to state of the art black-box solvers
- All of the above properties hold for non-continuous functions with non-linear constraints assuming the search space contains any sub-spaces that are Lipschitz smooth and convex

Objective function statement and nomenclature

Objective function statement i

Consider a general optimisation problem of the form

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

- Objective function maps an n-dimensional real space to a scalar value $f : \mathbb{R}^n \to \mathbb{R}$
- f can be either smooth or non-smooth depending on the local minimisation method used
- The variables $\mathbf{x}$ are assumed to be bounded
- $g_i(x)$ are the inequality constraints $\mathbf{g} : [\mathbf{l}, \mathbf{u}]^n \to \mathbb{R}^m$
- $h_j(x)$ are the equality constraints $\mathbf{h} : [\mathbf{l}, \mathbf{u}]^n \to \mathbb{R}^j$

Objective function statement ii

- It is assumed that the objective function has a finite number of local minima

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

$$\mathbf{x} \in \Omega \subseteq [\mathbf{l}, \mathbf{u}]^n \;=\; [l_1,\; u_1] \;\times\; [l_2,\; u_2] \;\times\; \ldots \;\times\; [l_n,\; u_n] \subseteq \mathbb{R}^n \tag{1}$$

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

$$\Omega = \{\mathbf{x} \in [\mathbf{l}, \mathbf{u}]^n \mid \mathbf{g}_i(\mathbf{x}) \geq 0, \forall i = 1, \ldots, m\} \tag{2}$$

When the constraints in **g** are linear the set Ω is always a compact space.

Introduction to homology groups of hypersurfaces

What is the homology group of a problem?

What is the homology group of a problem?

- Association of the (possibly non-manifold) search space with algebraic objects built on a homeomorphic topological space.
- Applied here to global optimisation theory mapping euclidean search spaces to a scalar value $f : \mathbb{R}^n \rightarrow \mathbb{R}$
- More generally shgo can be applied to calculate the homology groups of any real scalar field mapping on a manifold $\mathbb{M}^n$ $f : \mathbb{M}^n \rightarrow \mathbb{R}$

A brief one-dimensional motivation

A brief one-dimensional motivation i

Derivative free Lipschitz optimisation:

- f and g are black-box functions
- No derivative information available
- Assume Lipschitz constant is difficult to calculate

A brief one-dimensional motivation ii

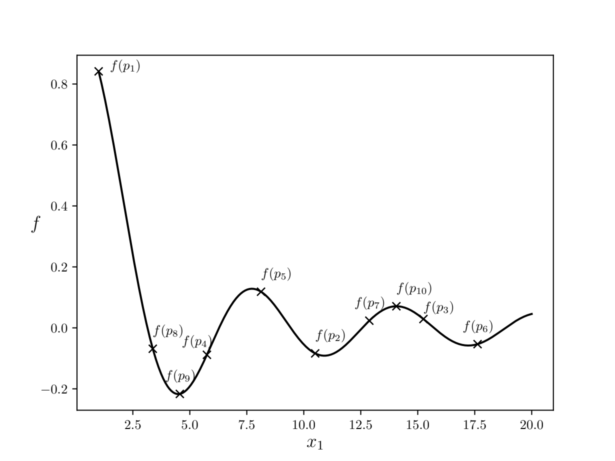


Figure 1: Sampling points on an objective function surface

A brief one-dimensional motivation iii

Number of minimisers $|\mathcal{M}^k| = 3$. How do we find the global minimum?

Popular approaches:

- Clustering algorithms using the Euclidean distance metric (topographical global optimisation (TGO) ([Henderson et al., 2015, Törn, 1986, Törn, 1990, Törn and Viitanen, 1992]), GLCCLUSTER etc.)
- Stochastic algorithms such as particle swarm optimisation (PSO) [Vaz and Vicente, 2009] and differential evolution (DE)
- Lipschitzian-based partitioning techniques using all possible Lipschitz constants in combined global and local searches (DIRECT (DIviding RECTangle) [Jones et al., 1993], DISIMPL (DIviding SIMPLices) [Paulavičius and Žilinskas, 2014], BB (Branch-and-bound) etc.)
- Approaches using affine geometric information (A-TGO)

A brief one-dimensional motivation iv

- There are many more classifications and algorithms available in literature. For an extensive review and experimental comparison of 22 derivative-free optimisation algorithms refer to [Rios and Sahinidis, 2013].
- From the conclusions in the study it can be observed that many of the most competitive commercial algorithms (TOMLAB) are those based on the DIRECT algorithm.
- The shgo algorithm is a new approach similar in some ways similar to DIRECT and DISIMPL in that geometric partitioning is used. However, instead using heuristics to switch between a local and a global search, the homology groups are calculated and its properties are used to circumvent the need for a local search phase.
- Algebraic topology theory is applied to provide rigorous convergence properties and higher performance properties.

Computing the homology groups of hypersurfaces

How do we compute the homology group of an optimisation problem?

Overview: from Lipschitz surfaces to homology groups and the solution(s) of optimisation problems

$$
\begin{tikzcd}
 & & \mathbf{H}_i(\mathcal{H}), \mathbf{H}_i(\mathcal{S}) \arrow[r, "\text{Eilenberg-Steenrod Axioms[1]}"] \arrow[dll, leftrightarrow, "\text{Simplicial homology}"'] \arrow[d, leftrightarrow, "\forall i(\mathbf{H}_i(\mathcal{H}) \cong \mathbf{H}_i(\mathcal{S}))"] & \text{Invariance} \arrow[d, "\text{Finite cardinality}"'] \arrow[dl, leftrightarrow] \\
\mathrm{f} \arrow[r, "h \circ f : \mathcal{P} \to \mathcal{H}"] & \mathcal{H} \arrow[r, leftrightarrow, "\mathcal{H} \cong \mathcal{K}", "k : \mathcal{K} \to \mathcal{S}"'] \arrow[dr, "\mathit{Sperner}"', "\partial C_i(\mathcal{H})"] & \mathcal{S} & f^*, \mathbf{x}^* \\
 & & \{\mathbf{x} | \forall x_i \leq \partial C(\mathcal{H}^k)(\mathbf{H}_i(\mathbf{x}) \geq 0)\} \arrow[r, "\text{DEC[2]}", "\text{MVT[3]}"'] & \nabla f(\mathbf{X}) = \bar{0} \arrow[u, "\text{Sets of solutions}"']
\end{tikzcd}
$$

1. [Eilenberg and Steenrod, 1952] , 2. Discrete exterior calculus , 3. (Discrete) Mean Value Theorem

Simplicial homology global optimisation

shgo: summary i

The algorithm itself consists of four major steps which will be described in detail:

1. Uniform sampling point generation of N vertices in the search space within the bounded and constrained subspace of Ω from which the $0-$chains of $\mathcal{H}^0$ are constructed
2. Construction of the directed simplicial complex $\mathcal{H}$ by triangulation of the vertices $h : \mathcal{P} \rightarrow \mathcal{H}$
3. Construction of the minimiser pool $\mathcal{M} \subset \mathcal{H}^0$ by repeated application of Sperner's lemma
4. Local minimisation using the starting points defined in $\mathcal{M}$

In the development of shgo we require several concepts from algebraic and combinatorial topology [Hatcher, 2002, Henle, 1979]. We will start with the basic building blocks of a simplicial complex:

Definition

A **k-simplex** is a set of $n+1$ vertices in a convex polyhedron 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 k-simplex is the set

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

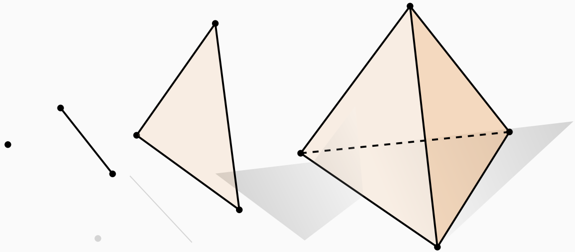


Figure 2: A 0-simplex (point), 1-simplex (edge), 2-simplex (triangle) and a 3-simplex (tetrahedron) (Figure adapted from [Keenan Crane, 2013])

Definition

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 $\mathcal{H}^k$.

Definition

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

Examples:

0-chain	**1-chain**	**2-chain**
A set of vertices	A set of edges	A set of triangles

shgo: nomenclature v

- $C(\mathcal{H}^k)$ 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 1-simplex in $\mathcal{H}^1$ from v_i to v_j then the symbol $\overline{v_i v_j}$ represents the 1-simplex
- This 1-simplex is bounded by the $0-$chain $\partial\left(\overline{v_i v_j}\right) = v_j - v_i$
- A 2-simplex 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 $\partial\left(\overline{v_i v_j v_j}\right) = \overline{v_i v_j} + \overline{v_j v_k} + \overline{v_j v_i}$.

Definition

The **star** of a vertex v_i, written $\mathrm{st}\left(v_i\right)$, is the set of points Q such that every simplex containing Q contains v_i.

The $k-$chain $C(\mathcal{H}^k), k = n + 1$ of simplices in $\mathrm{st}\left(v_i\right)$ forms a boundary cycle $\partial(C(\mathcal{H}^{n+1}))$ with $\partial\left(\partial(C(\mathcal{H}^{n+1}))\right) = \emptyset$. The faces of $\partial(\mathcal{H}^{n+1})$ are the bounds of the domain defined by $\mathrm{st}\left(v_i\right)$.

Simplicial homology global optimisation: $h : \mathcal{P} \rightarrow \mathcal{H}$

shgo: $h : \mathcal{P} \to \mathcal{H}$ i

$$
\begin{tikzcd}
& & \mathbf{H}_i(\mathcal{H}), \mathbf{H}_i(\mathcal{S}) \arrow[r, "\text{Eilenberg-Steenrod Axioms}"] \arrow[d, leftrightarrow, "\forall i(\mathbf{H}_i(\mathcal{H})\cong\mathbf{H}_i(\mathcal{S}))"] & \text{Invariance} \arrow[d, "\text{Finite cardinality}"'] \arrow[dl, leftrightarrow] \\
f \arrow[r, "h\circ f:\mathcal{P}\to\mathcal{H}"] & \mathcal{H} \arrow[ur, leftrightarrow, "\text{Simplicial homology}"] \arrow[r, leftrightarrow, "\mathcal{H}\cong\mathcal{K}", "k:\mathcal{K}\to\mathcal{S}"'] \arrow[dr, "\textit{Sperner}"', "\partial C_i(\mathcal{H})"] & \mathcal{S} & f^*, \mathbf{x}^* \\
& & \{\mathbf{x} | \forall x_i \leq \partial C(\mathcal{H}^k)(\mathbf{H}_i(\mathbf{x}) \geq 0)\} \arrow[r, "\text{DEC}", "\text{MVT}"'] & \nabla f(\mathbf{X}) = \bar{0} \arrow[u, "\text{Sets of solutions}"]
\end{tikzcd}
$$

shgo: $h : \mathcal{P} \rightarrow \mathcal{H}$ ii

We define the constructions used to build the simplicial complex on the hypersurface f from which we compute the homology groups.

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

Definition

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

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

shgo: $h : \mathcal{P} \to \mathcal{H}$ iii

Definition

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

Definition

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.

shgo: $h : \mathcal{P} \rightarrow \mathcal{H}$ iv

Definition

The set $\mathcal{H}^1$ is constructed by directing every edge in E. A vertex $v_i \in \mathcal{H}^0$ is the 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 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 any 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

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

Example

The Ursem01 function for two dimensions is defined as follows [Gavana, 2016]

$$\min f, \; x \in \Omega = [0, 9] \times [-2.5, 2.5]$$

$$f(\mathbf{x}) = -\sin(2x_1 - 0.5\pi) - 3\cos(x_2) - 0.5x_1$$

shgo: $h : \mathcal{P} \rightarrow \mathcal{H}$ vii

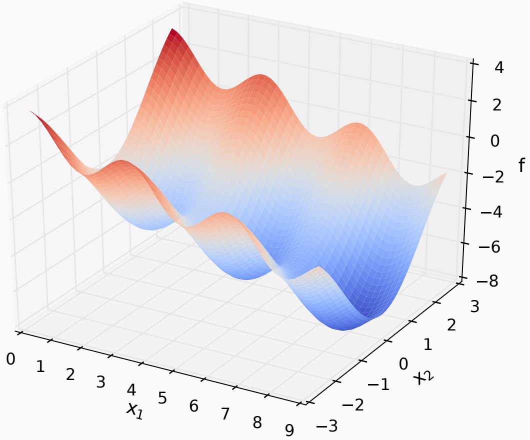


Figure 3: 3-dimensional plot of the Ursem01 function

shgo: $h : \mathcal{P} \rightarrow \mathcal{H}$ viii

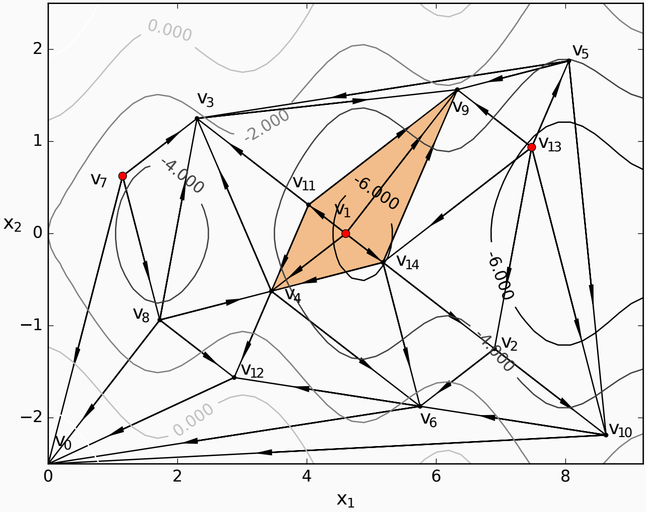


Figure 4: A directed complex $\mathcal{H}$ forming a simplicial approximation for an objective function. There are three minimiser vertices v_1, v_7 and v_{13} shown by the big red dots. The shaded area represents the domain defined by $\mathrm{st}\left(v_1\right)$

Simplicial homology global optimisation: locally convex sub-domains

shgo: locally convex sub-domains i

$$
\begin{tikzcd}
 & & \mathbf{H}_i(\mathcal{H}), \mathbf{H}_i(\mathcal{S}) \arrow[r, "\text{Eilenberg-Steenrod Axioms}"] \arrow[d, leftrightarrow, "\forall i(\mathbf{H}_i(\mathcal{H}) \cong \mathbf{H}_i(\mathcal{S}))"] & \text{Invariance} \arrow[d, "\text{Finite cardinality}"'] \\
\mathrm{f} \arrow[r, "h \circ f : \mathcal{P} \to \mathcal{H}"] & \mathcal{H} \arrow[ur, leftrightarrow, "\text{Simplicial homology}"] \arrow[r, leftrightarrow, "\mathcal{H} \cong \mathcal{K}", "k : \mathcal{K} \to \mathcal{S}"'] \arrow[dr, "\textit{Sperner} \quad \partial C_i(\mathcal{H})"] & \mathcal{S} \arrow[ur, leftrightarrow] & f^*, \mathbf{x}^* \\
 & & \{\mathbf{x} | \forall x_i \leq \partial C(\mathcal{H}^k)(\mathbf{H}_i(\mathbf{x}) \geq 0)\} \arrow[r, "\text{DEC}", "\text{MVT}"'] & \nabla f(\mathbf{X}) = \bar{0} \arrow[u, "\text{Sets of solutions}"]
\end{tikzcd}
$$

shgo: locally convex sub-domains ii

The shgo algorithm comes with a guarantee of stationary points in sub-domains near minimiser points

Theorem

*(**Stationary point in a minimiser star domain**) 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 $st(v_i)$.*

Overview of *proof:*

- Find a simplex with a Sperner labelling where each label represents a different $n+1$ label in every vector direction of the gradient vector field ∇f of f

shgo: locally convex sub-domains iii

- Of the $n+1$ Cartesian directions we require only a vector pointing towards a section defined by $n+1$ hyperplane cuts
- The remainder of the proof then proceeds as usual for Brouwer's fixed point theorem [Brouwer, 1911] found in for example [Henle, 1979, p. 40] utilising Sperner's lemma

Theorem

(**Sperner's lemma [Sperner, 1928]**) *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.*

- For any minimiser $v_i \in \mathcal{M} \subseteq \mathcal{H}^0$ we have by construction that for any vertex v_j with incidence on a connecting edge $\overline{v_i v_j}$ that $f(v_i) < f(v_j)$

shgo: locally convex sub-domains iv

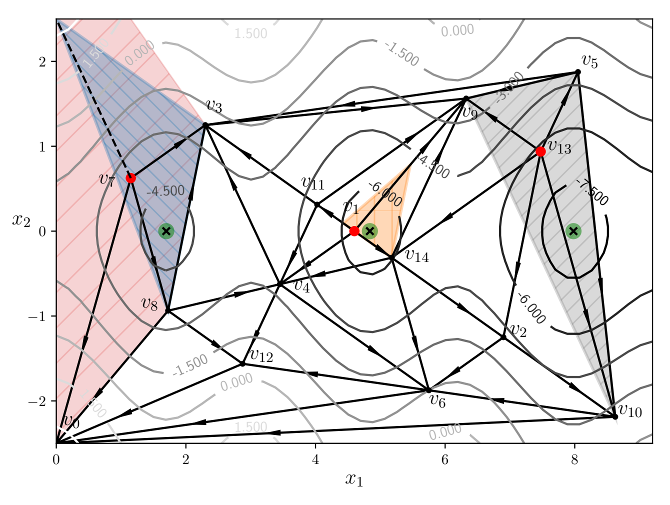
- By the MVT there is at least one point on $\overline{v_i v_j}$ where ∇f points towards a Cartesian direction in a section that can receive a unique Sperner label
- At this point are two possibilities:
  1. If we have $n+1$ vertices with incidence on an edge $\overline{v_i v_j} \subseteq \mathcal{H}^1$ in every required Cartesian direction then we have a simplex within $\mathrm{st}\,(v_i)$ with a complete Sperner labelling
  2. In the case where we do not have $n+1$ vertices in every required section then by construction there is no vertex between v_i and the boundary of f defined by Ω in the required section. The two possibilities are:
     - 2.1 In the case where the constraint is not active and there exists at least one point v_k boundary where ∇f does not point towards the boundary and by the MVT v_k can receive a unique Sperner label from which we can construct a simplex within $\mathrm{st}\,(v_i)$ with Sperner labelling
     - 2.2 In the case where the constraint is active a local minimum lies on the constraint which is in the domain defined $\mathrm{st}\,(v_i)$

shgo: locally convex sub-domains v

- Following the combinatorial version of Brouwer's fixed point theorem [Henle, 1979] since ∇f is continuous and the domain $\mathrm{st}\,(v_i)$ is compact we can produce a sequence of complete triangulations with arbitrarily small size in which the size of the simplices decreases toward zero
- This sequence produces a sequence of vertices with gradients $\nabla f(V)$ pointing in every $n+1$ direction. By continuity there is a vector $\nabla f(\mathbf{X})$ near the sequences, since the zero vector is the only vector pointing in all $n+1$ directions we have a point $\mathbf{X}$ bounded by the domain defined by $\mathrm{st}\,(v_i)$ where $\nabla f(\mathbf{X}) = \bar{0}$

This concludes the proof.

shgo: locally convex sub-domains vi



shgo: locally convex sub-domains vii

- The three circled crosses are the (approximate) minimima of the objective function within the given bounds.
- Here we have divided the plane so that the 3 required directions are $[0, \frac{\pi}{2})$, $[\frac{\pi}{2}, \pi)$ and $[\pi, 2\pi)$
- Note that this division is arbitrary and any $n + 1 = 3$ subdivisions can be chosen as long as all possible $n + 1 = 3$ directions can form a simplex in the space are covered (affinely independent)
- The three possible Sperner simplices are contained within the star domains of each minimiser $\mathrm{st}\,(v_1)$, $\mathrm{st}\,(v_7)$ and $\mathrm{st}\,(v_{13})$.
    1. v_7 is an example of a simplex without a complete Sperner labelling the red shaded area around v_7 is the bounded domain wherein at least one local minimum exist

2. v_{13} has three possible edges in $[\frac{\pi}{2}, \pi)$ on which a point exists that can be used as a vertex to receive a Sperner labelling for that direction namely $\overline{v_{13}v_{14}}$, $\overline{v_{13}v_{2}}$ and $\overline{v_{13}v_{10}}$. The only possible edges in the $[0, \frac{\pi}{2})$, $[\frac{\pi}{2}, \pi)$ directions are $\overline{v_{13}v_{5}}$ and $\overline{v_{13}v_{9}}$ respectively. The simplex $\overline{v_{5}v_{9}v_{10}}$ drawn in the figure is not necessarily the simplex with a Sperner labelling. The three vertices of the Sperner simplex which are proven to exist through the MVT exists on each of the edges $\overline{v_{13}v_{14}}$, $\overline{v_{13}v_{2}}$ and $\overline{v_{13}v_{10}}$ in a subdomain of this simplex $\overline{v_{5}v_{9}v_{10}}$
3. v_{1} for example the simplex surrounding the minimiser is a possible Sperner simplex with vertices on the edges in every required direction

shgo: locally convex sub-domains ix

- Note that if the edge $\overline{v_{13} v_{14}}$ was chosen instead of $\overline{v_{13} v_{10}}$ then the local minimum of the function would be outside the domain of the simplex with the Sperner labelling. This is an important observation because it demonstrates that the theorem cannot be used to further refine the location of the local minimum from the domain $\mathrm{st}\,(v_{13})$ using mechanisms of the proof, it only states that at least one local minimum exists within $\mathrm{st}\,(v_{13})$
- The boundaries of $\mathrm{st}\,(v_{13})$ can be found using the $3-$chain $C_{13}(\mathcal{H}^3)$ of simplices in $\mathrm{st}\,(v_{13})$, recall that the directions of simplices higher than dimension 2 are undefined and so the directions can be arbitrarily chosen

$$C_{13}(\mathcal{H}^3) = \overline{v_{13} v_{10} v_5} + \overline{v_{13} v_5 v_9} + \overline{v_{13} v_9 v_{14}} + \overline{v_{13} v_{14} v_2} + \overline{v_{13} v_2 v_{10}}$$

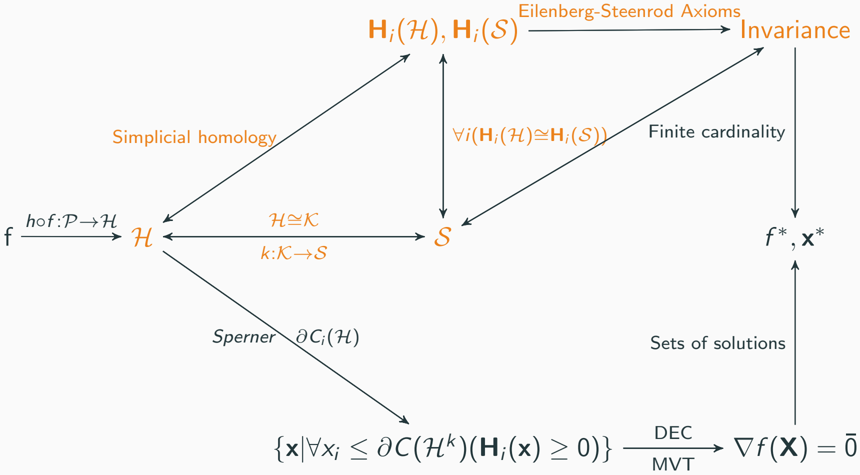
shgo: locally convex sub-domains x

- $C_{13}(\mathcal{H}^3)$ clearly forms a cycle, applying the boundary operator we find the faces defining the bounds of the domain of $\mathrm{st}\left(v_i\right)$ which in this case is the chain of edges with defined direction

$$\partial(C_{13}(\mathcal{H}^3)) = -\overline{v_{10}\, v_5} + \overline{v_5\, v_9} - \overline{v_9\, v_{14}} + \overline{v_{14}\, v_2} + \overline{v_2\, v_{10}}$$

thus $\partial\left(\partial(C(\mathcal{H}^3))\right) = \emptyset$

Simplicial homology global optimisation: invariance


$\mathbf{H}_i(\mathcal{H}), \mathbf{H}_i(\mathcal{S})$
Eilenberg-Steenrod Axioms
Invariance
Simplicial homology
$\forall i(\mathbf{H}_i(\mathcal{H}) \cong \mathbf{H}_i(\mathcal{S}))$
Finite cardinality
f
$h \circ f : \mathcal{P} \to \mathcal{H}$
$\mathcal{H}$
$\mathcal{H} \cong \mathcal{K}$
$k : \mathcal{K} \to \mathcal{S}$
$\mathcal{S}$
$f^*, \mathbf{x}^*$
Sperner
$\partial C_i(\mathcal{H})$
Sets of solutions
$\{\mathbf{x} | \forall x_i \leq \partial C(\mathcal{H}^k)(\mathbf{H}_i(\mathbf{x}) \geq 0)\}$
DEC
MVT
$\nabla f(\mathbf{X}) = \bar{0}$

shgo: invariance ii

Theorem

*(**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 $|\mathcal{M}|$**.*

Definition

Consider a simplicial complex $\mathcal{H}$ built on an objective function f with a compact feasible set Ω using Definitions 7 through 10. The surface is said to be **adequately sampled** if there is one and only one true stationary point within every domain defined by the stationary point theorem

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).

shgo: invariance iv

First we will prove invariance in the case where $\Omega = [\mathbf{l}, \mathbf{u}]^n$ (ie a compact space)

Overview of *proof* :

- The proof relies on a homomorphism between the simplicial complex $\mathcal{H}$ constructed in the bounded hyperrectangle Ω and the homology (mod 2) groups of a constructed surface $\mathcal{S}$ on which we can invoke the invariance theorem
- Define the n-torus $\mathcal{S}_0$ from the compact, bounded hyperrectangle Ω by identification of the opposite faces and all extreme vertices
- Now for every strict local minimum point $\mathbf{p} \in \Omega$ puncture a hypersphere and after appropriate identification the resulting n-dimensional manifold $\mathcal{S}_g$ is a connected g sum of g tori $S := S_0 \# S_1 \# \cdots \# S_{g-1} \qquad (g \text{ times})$

shgo: invariance v

- Any triangulation $\mathcal{K}$ of the topological space $\mathcal{S}$ is homeomorphic to $\mathcal{S}$,
$$\mathbf{H}_k(\mathcal{K}) \cong \mathbf{H}_k(\mathcal{S}) \; \forall k \subset \mathbb{Z}$$
- Note that this homomorphism is for a mod 2 homology between a triangulation $\mathcal{K}$ and the surface $\mathcal{S}$ and is thus undirected.
- A triangulation corresponding to all vertices and faces of $\mathcal{K}$ can be directed according to the first 3 definitions for h providing the directed simplicial complex $\mathcal{H}$
- By construction we have, for an adequately sampled simplicial complex $\mathcal{H}$, an equality which exists between the cardinality of $\mathcal{M}$ and the Betti numbers of $\mathcal{S}$ as

$$|\mathcal{M}| = h_1 = \mathrm{rank}(\mathbf{H}_1(\mathcal{S})) = \mathrm{rank}(\mathbf{H}_1(\mathcal{K}))$$

- Here we invoke the invariance theorem

Theorem

*(**Invariance theorem [Henle, 1979]**) The homology groups associated with a triangulation $\mathcal{K}$ of the a compact, connected surface $\mathcal{S}$ are independent of $\mathcal{K}$. In other words, the groups $\mathbf{H}_0(\mathcal{K})$, $\mathbf{H}_1(\mathcal{K})$ and $\mathbf{H}_2(\mathcal{K})$ do not depend on the simplices, incidence coefficients, or anything else arising from the choice of the particular triangulation $\mathcal{K}$; they depend only on the surface $\mathcal{S}$ itself.*

- The invariance theorem can be extended to higher dimensional triangulable spaces using singular homology through the Eilenberg-Steenrod Axioms [Eilenberg and Steenrod, 1952, Henle, 1979]

shgo: invariance vii

- As a direct consequence any triangulation of $\mathcal{S}$ will produce the same homology groups for $\mathcal{K}$
- Adding any new sampling point within the corresponding subdomains of $\mathrm{st}\,(v_i)\ \forall i(v_i \in \mathcal{M} \subseteq \mathcal{H}^0)$ as defined in the stationary point theorem will by the first 4 definitions of h need to be connected directly to v_i by a new edge or the triangulation is no longer a simplicial complex and thus not increase $|\mathcal{M}|$ since only one vertex will be the new minimiser
- After adding any sampling point outside a domain $\mathrm{st}\,(v_i)$ then, through the established homomorphism, any construction of $\mathcal{H}$ will produce the same homology groups since $\mathrm{rank}(\mathbf{H}_1(\mathcal{K}))$ remains unchanged and it is thus not possible for a new vertex to be wrongly identified as a minimiser in the triangulation $\mathcal{H}$

shgo: invariance viii

This conclues the proof that any increase in N will not further increase $|\mathcal{M}|$.

N.B.

Any further refinement in the simplicial complex by further sampling does not increase the number of locally convex sub-domains in a compact space!

shgo: invariance ix

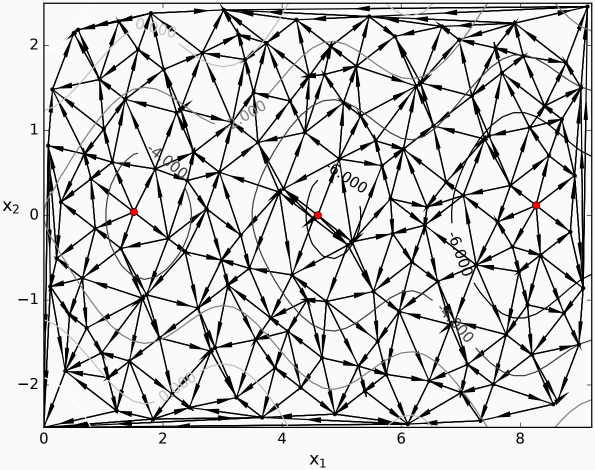


Figure 5: Further refinement of the simplicial complex from the example problem does increase the number of locally convex sub-domains extracted by shgo

shgo: invariance xi

Finally we prove a stronger invariance and convergence

- Consider the case where the constraints **g** are non-linear
- In addition we allow the objective function f to be non-continuous and non-linear
- It is still assumed that the variables **x** are bounded
- Furthermore we assume that there is a feasible solution so that $\Omega \neq \emptyset$ and that there exists at least point in range of f mapped within the domain Ω
- We will prove that if the simplicial sampling sequence [Endres, 16] is used, then shgo-simplicial will **retain the Invariance property**
- Secondly **convergence** of the shgo algorithm to the global minimum is proved if the sub-triangulation simplicial sampling sequence is used

shgo: invariance xii

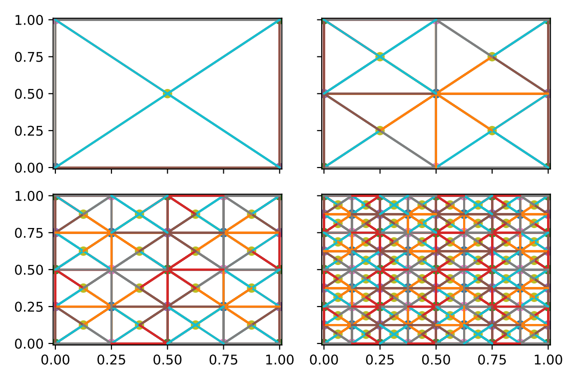


Figure 6: Simplicial sampling by sub-triangulation of hyper-rectangles

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

Definition

For an objective function f, $\mathcal{F}$ is the set of scalar outputs mapped by the objective function $f : \mathcal{P} \rightarrow \mathcal{F}$ 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 $f : v_i \rightarrow \infty$.

Note 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.

Theorem

*(**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 $|\mathcal{M}|$**.*

Overview of *proof* :

- The compact invariance theorem 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 compact Invariance property
- 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 $\mathcal{K}_i$

shgo: invariance xvii

- 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 the compact Invariance theorem
- Any point that is not in Ω is not connected to any graph structure by the definitions in h and therefore cannot increase the rank of any homology group $\mathbf{H}_1(\mathcal{K}_i)$

shgo: invariance xviii

- Finally any vertex $v_i \in \Omega$ for which $f(v_i)$ does not exist will by the new infinity construction for h be mapped to infinity by the defined mapping $f : v_i \rightarrow \infty$
- By the definition, v_i can not be a minimiser and therefore cannot increase the rank of any homology group $\mathbf{H}_1(\mathcal{K}_i)$
- 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 convergence proof used by [Paulavičius et al., 2014] for subdivided simplicial complexes

Proposition

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 $\left\|\mathbf{x}_i^k - \mathbf{x}\right\| < \epsilon$.

shgo: invariance xix

- Sampling points $\mathbf{x}_i$ are vertices $\mathcal{H}^0$ belonging to the set of n-dimensional simplices $\mathcal{H}^n$
- Let δ^k_{max} be the largest diameter of the largest simplex
- Since the subdivision is symmetrical all simplices have the same diameter δ^k_{max} 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 concluses the proof.

Convergence

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 the stationary point theorem applies to any minimiser in $\mathbb{B}_i$. In practice the definition of h is implemented in [Endres, 16] by using exception handling that can capture any mathematical errors in addition to converting any none float numbers outputted by an objective function to infinity objects.

But why?

$$
\begin{tikzcd}
 & & \mathbf{H}_i(\mathcal{H}), \mathbf{H}_i(\mathcal{S}) \arrow[r, "\text{Eilenberg-Steenrod Axioms}"] \arrow[d, leftrightarrow, "\forall i(\mathbf{H}_i(\mathcal{H}) \cong \mathbf{H}_i(\mathcal{S}))"] & \text{Invariance} \arrow[d] \arrow[dl, leftrightarrow, "\text{Finite cardinality}"] \\
\mathrm{f} \arrow[r, "h \circ f : \mathcal{P} \to \mathcal{H}"] & \mathcal{H} \arrow[ur, leftrightarrow, "\text{Simplicial homology}"] \arrow[r, leftrightarrow, "\mathcal{H} \cong \mathcal{K}", "k : \mathcal{K} \to \mathcal{S}"'] \arrow[dr, "\text{Sperner}"', "\partial C_i(\mathcal{H})"] & \mathcal{S} & f^*, \mathbf{x}^* \\
 & & \{\mathbf{x} | \forall x_i \leq \partial C(\mathcal{H}^k)(\mathbf{H}_i(\mathbf{x}) \geq 0)\} \arrow[r, "\text{DEC}", "\text{MVT}"'] & \nabla f(\mathbf{X}) = \bar{0} \arrow[u, "\text{Sets of solutions}"]
\end{tikzcd}
$$

shgo: algorithm ii

procedure INITIALISATION
  Input an objective function f, constraint functions $\mathbf{g}$ and variable bounds and $[\mathbf{l}, \mathbf{u}]^n$.
  Input N initial sampling points.
  Define a sampling sequence that generates a set $\mathcal{X}$ of sampling points in the unit hypercube space $[\mathbf{0}, \mathbf{1}]^n$
  Define the empty set $\mathcal{M}^E = \emptyset$ of vertices evaluated by a local minimisation.
end procedure
while $\mathbf{TERM}(\mathbf{H}_1(\mathcal{H}), \min\{\mathcal{F}\})$ is False **do**
  procedure SAMPLING
    $\mathcal{P} = \emptyset$
    while $|\mathcal{P}| < N$ **do**
      Generate $N - |\mathcal{P}|$ sequential sampling points $\mathcal{X} \subset \mathbb{R}^n$
      Stretch $\mathcal{X}$ over the lower and upper bounds $[\mathbf{l}, \mathbf{u}]^n$

shgo: algorithm iii

$\mathcal{P} = \{\mathcal{X}_i \mid \mathbf{g}(\mathcal{X}_i) \geq 0, \forall \mathcal{X}_i \in \mathcal{X}\} \cup \mathcal{P}$ ▷ (Find $\mathcal{P}$ in the feasible subset Ω by discarding any points mapped outside the linear constraints g and adding to the current set of $\mathcal{P}$.)

Set $\mathcal{X} = \emptyset$

end while

Find $\mathcal{F}$ from the objective function $f : \mathcal{P} \rightarrow \mathcal{F}$ for any new points in $\mathcal{P}$

end procedure

procedure CONSTRUCT/APPEND DIRECTED COMPLEX $\mathcal{H}$

Calculate $\mathcal{H}$ from $h : \mathcal{P} \rightarrow \mathcal{H}$ ▷ (If $\mathcal{H}$ was already constructed new points in $\mathcal{P}$ are incorporated into the triangulation.)

Calculate $\mathbf{H}_1(\mathcal{H})$

end procedure

procedure CONSTRUCT $\mathcal{M}$

Find $\mathcal{M}$ from the definitions of h.

shgo: algorithm iv

24: **end procedure**

25: **procedure** Local minimisation

26: Calculate the approximate local minima of f using a local minimisation routine with the elements of $\mathcal{M} \setminus \mathcal{M}^E$ as starting points. ▷ Process the most promising points first.

27: $\mathcal{M}^E = \mathcal{M}^E \cap \mathcal{M}$ ▷ This excludes the evaluation any element $v_i \in \mathcal{M}$ that is known to be the only point that in the domain $\partial \mathrm{st}(v_j)$ where v_j is known to any point already used as a starting point in Step 27. If any new $v_i \in \mathcal{M}$ not in $\mathcal{M}^E$ is known to be the only point $\partial \mathrm{st}(v_j)$ it can also be excluded.

28: Add the function outputs of the local minimisation routine to $\mathcal{F}$

29: **end procedure**

30: Find new value of $\mathbf{TERM}(\mathbf{H}_1)(\mathcal{H}, \min\{\mathcal{F}\})$

31: **end while**

shgo: algorithm v

procedure PROCESS RETURN OBJECTS

  Order the final outputs of the minima of f found in the local minimisation step to find the approximate global minimum.

end procedure

return the approximate global minimum and a list of all the minima found in the local minimisation step.

Experimental results

Open-source black-box algorithms i

- Here we compare shgo with the following algorithms:
  - topographical global optimization (TGO) [Henderson et al., 2015]
  - basinhopping (BH) [Li and Scheraga, 1987, Wales, 2003, Wales and Doye, 1997, Wales and Scheraga, 1999]
  - differential evolution (DE) [Storn and Price, 1997]
- BH and DE are readily available in the SciPy project [Jones et al., 01]
- BH is commonly used in energy surface optimisations [Wales, 2015]
- DE has also been applied in optimising Gibbs free energy surfaces for phase equilibria calculations [Zhang and Rangaiah, 2011]
- SciPy global optimisation benchmarking test suite [Adorio and Dilman, 2005, Gavana, 2016, Jamil and Yang, 2013, Mishra, 2007, Mishra, 2006, NIST, 2016]

Open-source black-box algorithms ii

- The test suite contains multi-modal problems with box constraints, they are described in detail in `http://infinity77.net/global_optimization/` Link
- The stochastic algorithms (BH and DE) used the starting points provided by the test suite.
- Stopping criteria $pe = 0.01\%$
- For every test the algorithm was terminated if the global minimum was not found after 10 minutes of processing time and the test was flagged as a fail.
- For comparisons we used normalised performance profiles [Dolan and Moré, 2002] using function evaluations and processing time as performance criteria.
- In total 180 test problems were used.

Open-source black-box algorithms iii

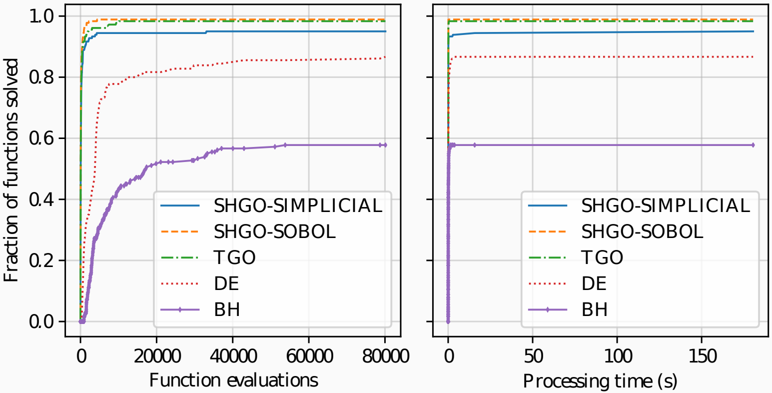


Figure 7: Performance profiles for SHGO, TGO, DE and BH

Open-source black-box algorithms iv

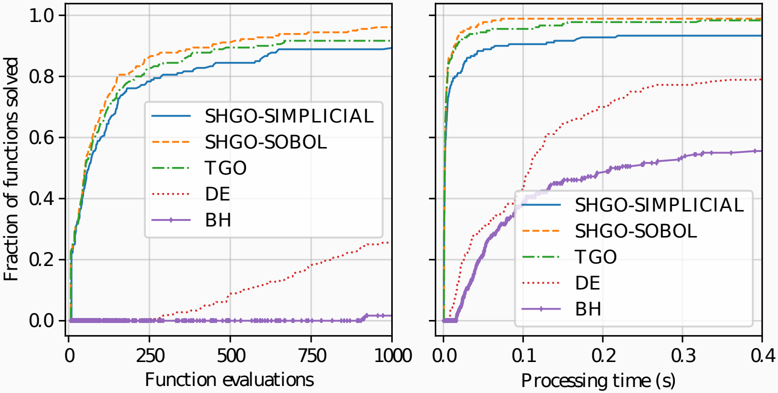


Figure 8: Performance profiles with ranges f.e. = [0, 1000] and p.t. = [0, 0.4]

Open-source black-box algorithms v

- shgo-sobol was the best performing algorithm
- ... followed closely by tgo and shgo-simpl
- shgo-sobol tends to outperform tgo, solving more problems or a given number of function evaluations as expected for the same sampling point sequence.
- tgo produced more than one starting point in the same locally convex domain while shgo is guaranteed to only produce one after adequate sampling
- While shgo-simpl has the advantage of having the theoretical guarantee of convergence, the sampling sequence has not been optimised yet requiring more function evaluations with every iteration than shgo-sobol.

Linear-constrained optimisation problems i

- The DISIMPL algorithm was recently proposed by [Paulavičius and Žilinskas, 2014]
- The experimental investigation shows that the proposed simplicial algorithm gives very competitive results compared to the DIRECT algorithm [Paulavičius and Žilinskas, 2016]
- More recently the Lc-DISIMPL variant of the algorithm was developed to handle optimisation problems with linear constraints [Paulavičius and Žilinskas, 2016]
- Test on 22 optimisation problems again using the stopping criteria $pe = 0.01\%$
- Lc-DISIMPL-v, PSwarm (avg), DIRECT-L1 results produced by [Paulavičius and Žilinskas, 2016]

Linear-constrained optimisation problems ii

Table 1: Performance over all 22 test problems.

problem	algorithm	f.e.	runtime (s)
Average	SHGO-simplicial	65	0.012852
	SHGO-sobol	88	0.004144
	TGO	100	0.004542
	Lc-DISIMPL-v	366	-
	Lc-DISIMPL-c	$>$5877	-
	PSO (avg)	3011	-
	DIRECT-L1 ($pp = 10$)	$>$17213	-
	DIRECT-L1 ($pp = 10^2$)	$>$28421	-
	DIRECT-L1 ($pp = 10^6$)	$>$75113	-

Linear-constrained optimisation problems iii

Table 2: Performance over all 22 test problems.

problem	algorithm	f.e.	nlmin	nulmin	runtime (s)
All	shgo-simpl	1463	26	26	0.27294
	shgo-sobol	1864	23	23	0.11225
	tgo	2123	29	25	0.093607

Linear-constrained optimisation problems iv

- The higher performance of shgo compared to tgo and DISIMPL is due to homological identification of unique locally convex sub-spaces
- shgo had
  - no wasted local minimisations unlike tgo because the locally convex sub-spaces are proven to be unique
  - no need for switching between a local and global step as in DISIMPL because the homology group rank growth tracks the global progress every iteration without requiring further refinement in sub-spaces
- For the full table of results see `https://stefan-endres.github.io/shgo/files/table.pdf`
  ▸ Link

Conclusions

Conclusions i

- The shgo algorithm shows promising properties and performance
- On test problems with linear constraints it was shown to provide competitive results to the TGO, Lc-DISIMPL, PSwarm and DIRECT-L1 algorithms
- On black-box problems it was shown to provide competitive results to the TGO, BH and DE algorithms
- The use of a simplicial complex provides access to a wealth of tools from combinatorial topology and the growing field of computational homology. It is hoped that these will drive further extensions and development

Conclusions ii

- Due to the useful characterisations of objective function hypersurfaces provided by the homology groups of the simplicial complex, shgo allows an optimisation practitioner with a useful visual tool for understanding and efficiently solving higher dimensional black and grey box optimisation problems
- It is especially appropriate for computationally expensive black and grey box functions common in science and engineering
- In addition because the homology groups can be calculated as sampling progresses an optimisation practitioner can both visualise the extent of the optimisation problems multi-modality and use intelligent stopping criteria for the sampling stage.

Thank you for your time.

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Questions?

Backup slides: References to obscure theorems and other additional information sources i

- Discrete MVT: https://www.sciencedirect.com/science/article/pii/S0377221707009952

Backup slides: Backup figures i

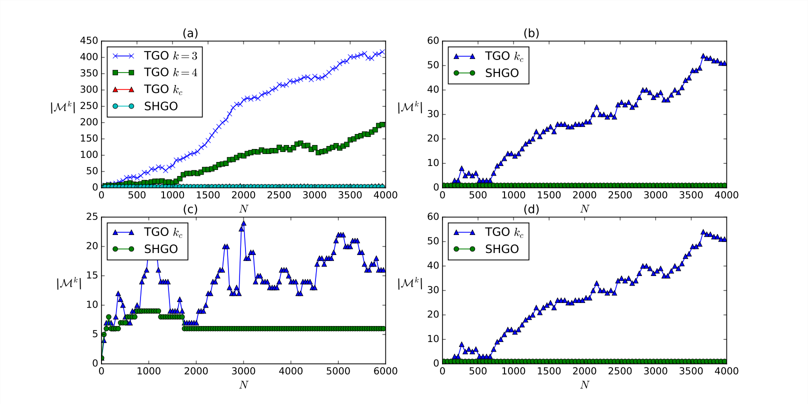

Figure 9: Invariance of homology groups after adequate sampling