Simplicial Homology Global Optimisation

A simplicial homology algorithm for Lipschitz optimisation

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This presentation is intended for an audience of professionals from a diverse set of backgrounds at the 2018 INFORMS Annual Meeting. For researchers and experts with a strong background in optimisation theory and applied mathematics a more detailed presentation can be found at https://stefan-endres.github.io/shgo/files/shgo_slides.pdf ▸ Link

Introduction

Introduction

- The simplicial homology global optimisation (shgo) algorithm is a general purpose global optimisation algorithm
- Appropriate for global optimisation of derivative free optimisation problems (DFO)
  - In DFO problems either the gradients of the functions are unavailable or the functions are black-box functions
- Applications limited to low dimensional problems ($\sim$10 dimensions)
- Information extracted by shgo in the limits:
  - Finds the global minimum (ex. "best" solutions, stable equilibrium)
  - Finds all other solutions (ex. other global minima, corresponding to quasi-equilibrium states that have physical meaning)
  - Quantifies the extent of global exploration of the objective function's surface using ideas from modern algebraic topology

Introduction: objective function statement i

Consider a general optimisation problem of the form

$$\begin{aligned} \text{minimize} \quad & f(\mathbf{x}),\ \text{by varying } \mathbf{x} \in \mathbb{R}^n \\ \text{subject to} \quad & g_i(\mathbf{x}) \geq 0,\ \forall i = 1, \dots, m \\ & h_j(\mathbf{x}) = 0,\ \forall j = 1, \dots, p \end{aligned}$$

- The objective function maps an n-dimensional real space to a scalar value $f : \mathbb{R}^n \to \mathbb{R}$
- 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 $\mathbf{h} : [\mathbf{l}, \mathbf{u}]^n \to \mathbb{R}^j$
- It is assumed that the objective function has a finite number of local minima

Introduction: objective function statement ii

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 $\mathbf{g}$ are linear the set Ω is always a compact space.

Applying simplicial homology theory in global optimisation: a brief one-dimensional motivation

A brief one-dimensional motivation i

Derivative free optimisation:

- f and g are expensive black-box functions
- No derivative information available or difficult to compute
- Common strategies in global optimisation hit the maps f and g with sampling points and use the resulting geometric information of the surfaces
- Many popular approaches are based on some kind of statistical or geometric reasoning or even more simply a multi-start routine that simply passes any promising sampling points to a local minimization routine

A brief one-dimensional motivation ii

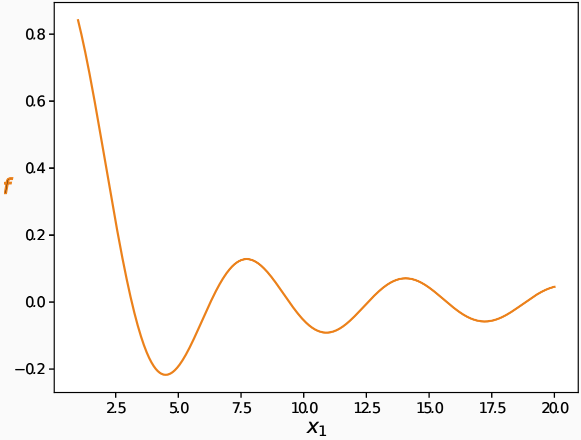


Figure 1: A 1-dimensional objective function surface $f : \mathbb{R}^1 \to \mathbb{R}$

A brief one-dimensional motivation iii

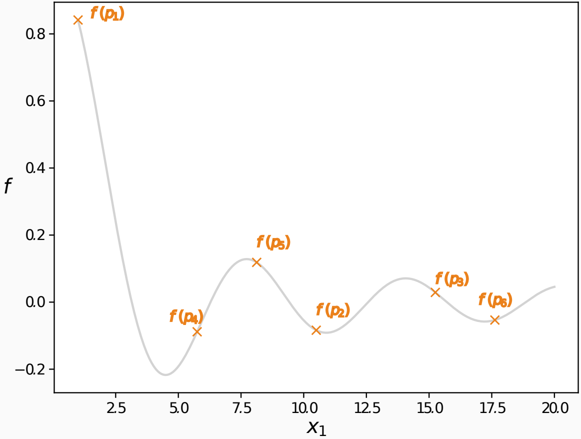


Figure 2: Sampling points on the surface found by hitting the map $f : \mathbb{R}^1 \to \mathbb{R}$

A brief one-dimensional motivation iv

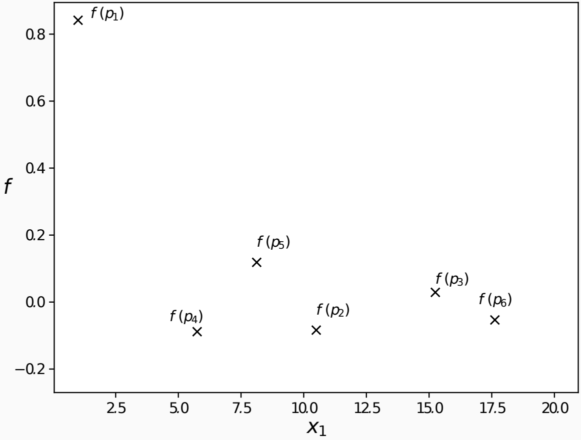


Figure 3: The information available to an algorithm (not very clear!)

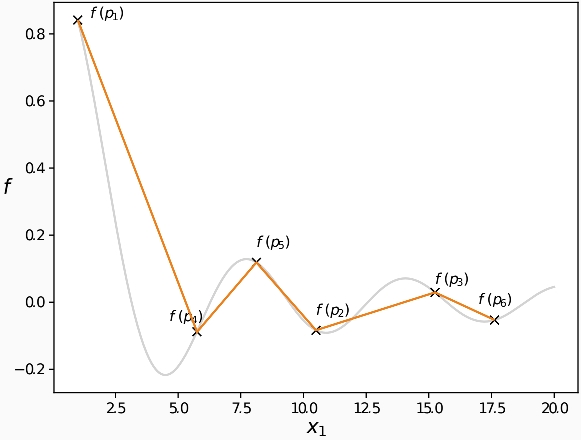


Figure 4: (Incomplete) geometric information found by building edges

A brief one-dimensional motivation vi

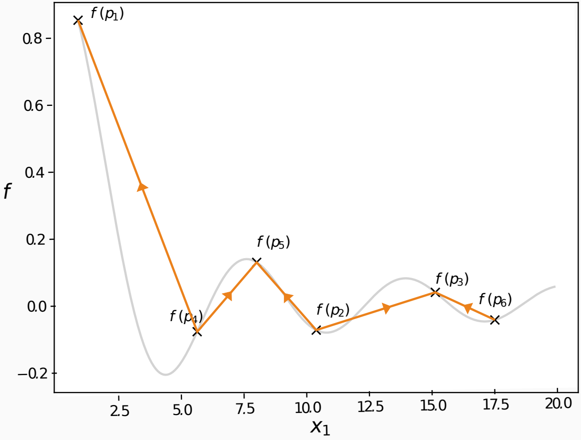


Figure 5: Directing the edges deduces even more information

A brief one-dimensional motivation vii

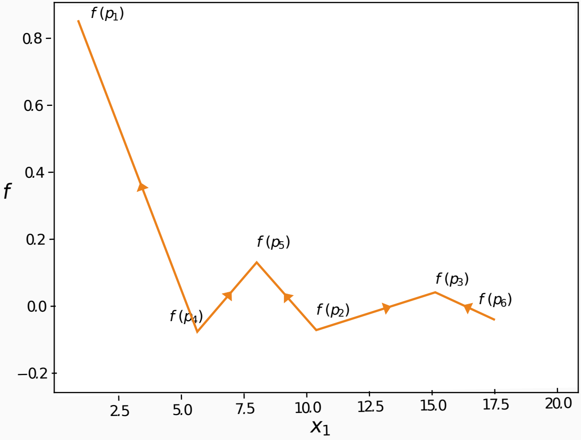


Figure 6: This geometric structure leaves us with a clearer picture

A brief one-dimensional motivation viii

- The number of local minima is at least 3 (by the mean value theorem)
- If we had just one fewer sampling point it would be impossible to deduce that there are 3 local minima
- On the other had if we had many more sampling points the number of minimisers would still only be 3 (a geometric **invariance!**)
- We want an idea of how many sampling points we need to find all solutions
- We would also like to know if these solutions are close together or far apart etc.
- We want to identify regions where it is proven we will find solutions (**locally convex sub-domains** that can be used in local-minimisation)
- Finally we want to extend these ideas to higher dimensions

Theoretical results in brief

Theoretical results in higher dimensions

- Use special simplicial complexes to extract information about the objective function (hyper-)surface
- Homology groups computed from sampling points on the hypersurface of objective functions allow us to deduce geometric features of the hypersurface that we can't visualize (a hypersurface has a dimension higher than 3)
- Algebraic topology theory is applied to provide rigorous **convergence** properties and higher performance properties by connecting convergence to the global minimum to geometric **invariance**
- Modern generalisations of Sperner's Lemma for the detection and computation of **locally convex sub-domains**
- Results have been rigorously extended to arbitrary dimensions[1]

[1] Detailed results can be found in the associated JOGO paper [Endres et al., 2018b]

Theoretical results in higher dimensions i

- **Locally convex sub-domains** can be found rigorously and the domains explicitly computed to pass to the local minimisation routine using the concept of star domains:

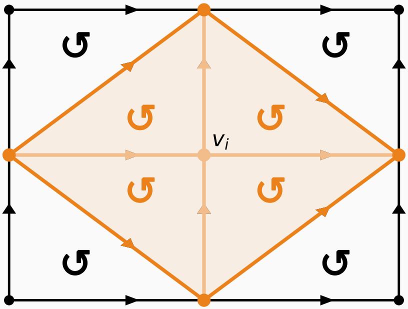
Definition

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.

- This concept replaces the one-dimension intervals from earlier, the shgo algorithm extracts $\mathrm{st}\left(v_i\right)$ domains from the data structures that are proven to contain local minima

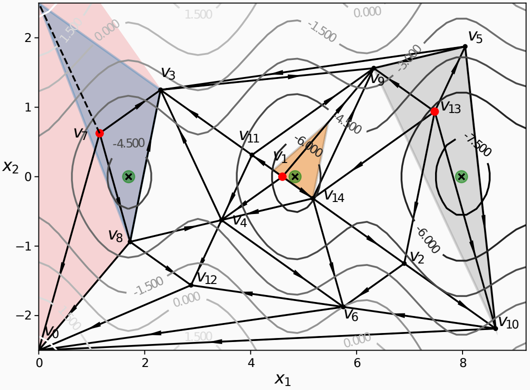
Theoretical results in higher dimensions ii

- The star domain defined by $\mathrm{st}\,(v_i)$
- The **boundary of the star domain** $\partial\mathrm{st}\,(v_i)$

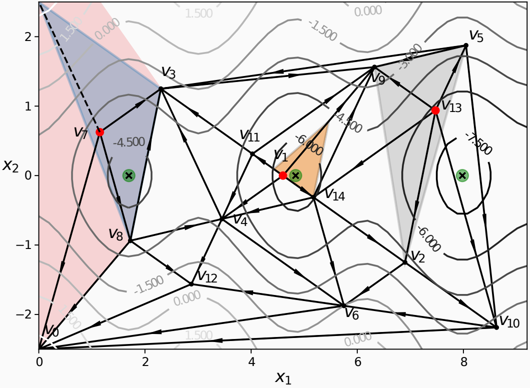


Theoretical results in higher dimensions iii

Possible Sperner simplices around domain v_7, domain v_1 and v_{13}



The domain $\partial(v_{13})$ cannot be further refined by the theorem



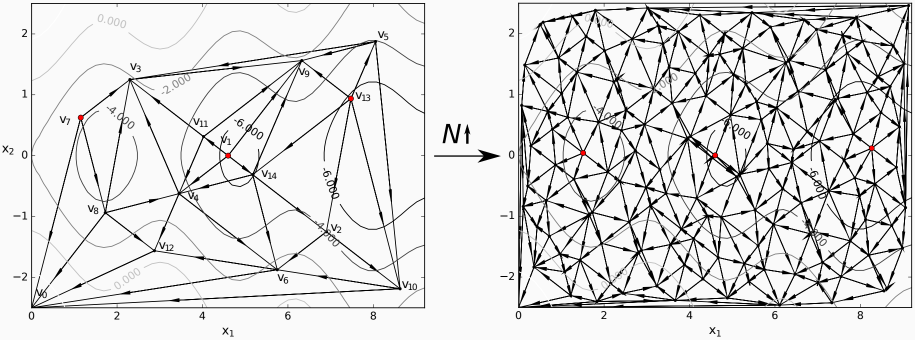


Figure 7: Further refinement of the simplicial complex doesn't increase the number of locally convex sub-domains extracted by shgo because of the homomorphims between the homology groups of $\mathcal{H}$ and $\mathcal{K}$

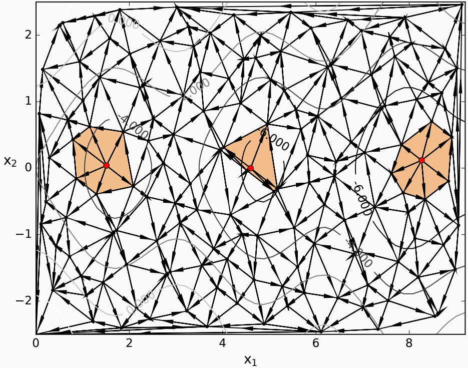


Figure 8: After increasing the number of sampling points the number of locally convex sub-domains from the example problem are still 3, however, the boundaries of the star domains have been further refined

Experimental results in brief

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	0.091168
	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

Open-source black-box algorithms i

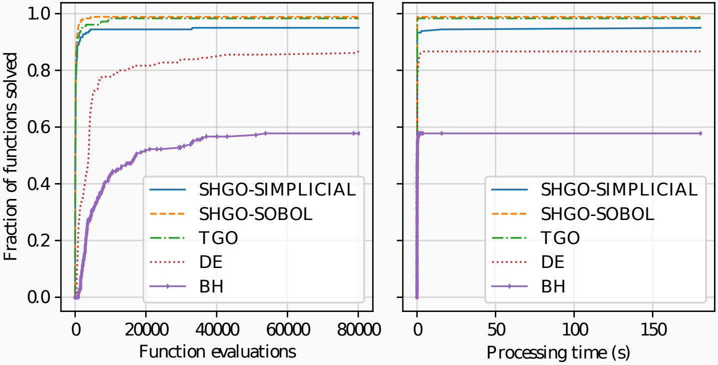


Figure 9: Normalized performance profiles for SHGO, TGO, DE and BH

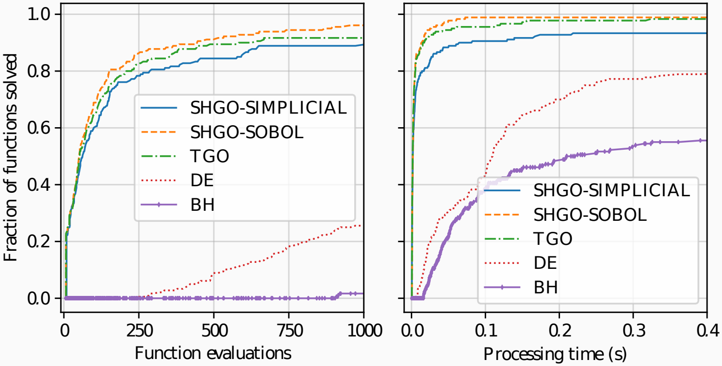


Figure 10: Performance profiles with ranges f.e. = [0, 1000] and p.t. = [0, 0.4]

Concluding remarks and future work

Conclusion and future work i

In conclusion:

- The shgo algorithm shows promising properties and competitive performance

Future:

- Many of the theoretical results apply to a wide range of spatial partitioning algorithms ex. the family of algorithms based on DIRECT, Branch-and-Bound etc.
- Global convergence proofs for these algorithms beyond continuous and Lipschitz smooth (discontinuous) objective functions [Endres et al., 2018a]

Thank you for your time.

Questions?

References

References i

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