Infinite dimensional optimistic optimisation with application on physical systems

Introduction

- Optimisation algorithms to optimise black-box functions with minimal number of evaluations is an active field of research.
- Simultaneous Optimistic Optimization (SOO) is one of the algorithm that is guaranteed to achieve the global maximum of a function within a bounded area without any prior assumptions on the function.
- In physical systems, there are several problems that require optimisation of functionals instead of function, for example, "what is the shape of trajectory of a ball to reach some points in the shortest amount of time?"
- Here we present an extension of SOO to optimise functionals or infinite dimensional optimisation.

Problem statement

Consider a 1D function, $f : \mathcal{X} \to \mathcal{F}$ where $\mathcal{X}, \mathcal{F}$ are bounded in $\mathbb{R}$ with fixed end points. It is an input of a functional $J : \mathcal{F}^{\mathcal{X}} \to \mathbb{R}$. Find

$$f_* = \arg\max_{f \in \mathcal{F}^{\mathcal{X}}} J[f]$$

Method

Simultaneous Optimistic Optimization (SOO)[1]

- SOO is a tree-based search algorithm which partitions the search space into several cells.
- Initially, there is only one cell which contains all the search space and the central point of the cell is evaluated. This is the tree's root.
- The cell is then divided into K smaller cells and their central points are evaluated. The smaller cells are children of the divided cell.

Algorithm 1 Simultaneous Optimistic Optimisation (SOO)

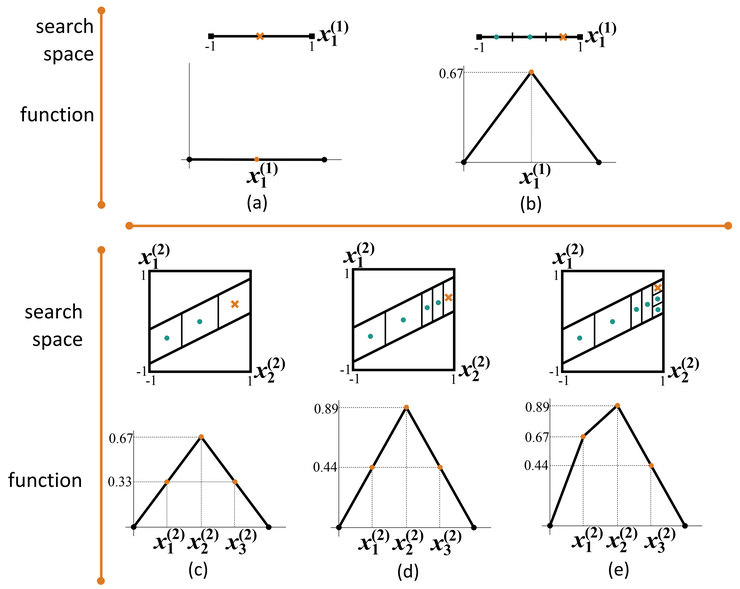
$\mathcal{T} \leftarrow (0, 0)$; $n \leftarrow 0$;
$\mathcal{L}_\mathcal{T}$:= any nodes in $\mathcal{T}$ without children
repeat
  $v_{max} \leftarrow 0$
  for $h \leftarrow 0$ **to** $\min(depth(\mathcal{T}), h_{max}(n))$ **do**
    $(h, i) \leftarrow \arg\max_{(h,j) \in \mathcal{L}_\mathcal{T}} f(x_{h,j})$
    if $v_{max} \leq f(x_{h,i})$ **then**
      Expand (h, i) to K children,
      evaluate the values of the children,
      and add them to $\mathcal{T}$
      $v_{max} \leftarrow f(x_{h,i})$; $n \leftarrow n + K$
    end if
  end for
until any stopping conditions
return $x_n^+ \leftarrow \arg\max_{(h,i) \in \mathcal{T}} f(x_{h,i})$

- The algorithm checks for every level in the tree. If a cell has a centre value larger than any cells with larger or the same size, then the cell is divided.
- The process is repeated until any stopping conditions reached.

Multi Level SOO (ML-SOO)

- ML-SOO starts with one dimensional search space, which denotes the position of the middle point between two end points. Also initialise l=1.
- Cells are divided according to SOO algorithm until all the widths are less than or equal to p^{-l}.
- If a cell has all widths less than or equal to p^{-l}, then add 2^l new dimensions with width p^{-l}. The new dimensions correspond to 2^l newly added points in the middle of previous points. Update $l = l + 1$.
- A cell is divided along the longest dimension, or if there are more than one dimensions with the same width, the 'oldest' dimension is divided first.
- If a cell is divided along the 'old' dimension, the position in 'newer' dimension around it is also changed.

Illustration of the algorithm



(a) It starts with one dimension, $x_1^{(1)}$, and the position of $x_1^{(1)}$ is 0.
(b) The cell is divided to 3 smaller cells. The function at ✖ on the search space is shown at the bottom, where $x_1^{(1)}$= 0.67.
(c) All cells now has width of 1/3 of the initial width, so two new dimensions are added in the search space, and two new points are added in the function. The 'old' dimension is $x_2^{(2)}$ while the 'newer' dimensions are $x_1^{(2)}$ and $x_3^{(2)}$.
(d) The rightmost cell is divided along the 'old' dimension, $x_2^{(2)}$, and also changes the position of $x_1^{(2)}$ and $x_3^{(2)}$.
(e) A cell is divided along a 'new' dimension, $x_1^{(2)}$, and it does not change other dimensions' positions.

Numerical experiments

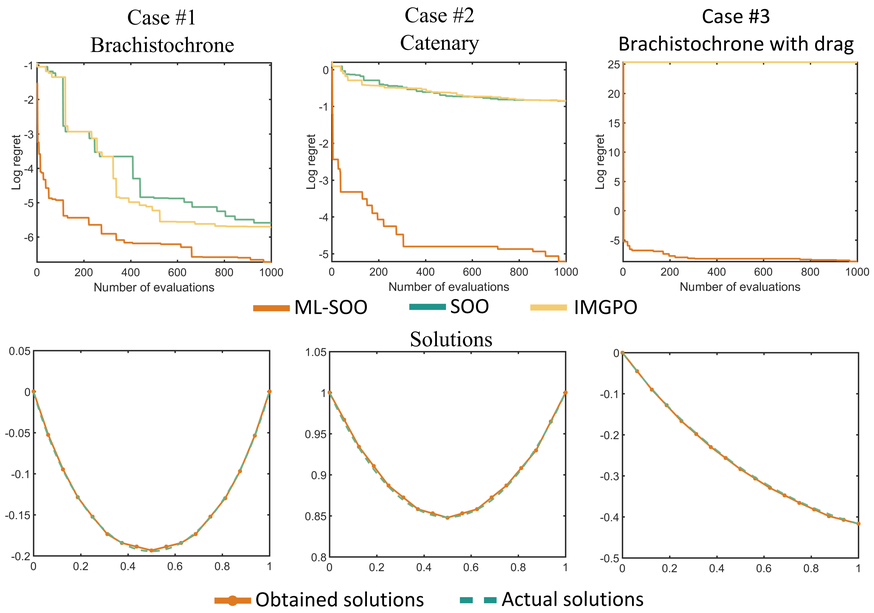
Cases

1. **Brachistochrone**: shape of the fastest path with gravity g=1 from point (0,0) to point (1,0) with initial velocity 0.624,
2. **Catenary**: shape of the minimum surface area of path between (0,1) to (1,1) if it is rotated along x-axis,
3. **Brachistochrone with drag**: shape of the fastest path with gravity g=1 and linear drag, F=-(0.02)v from point (0,0) to (1,0.417) with initial velocity 1.19.

Tested algorithms

1. Our algorithm, Multi-level Simultaneous Optimistic Optimization (**ML-SOO**)
2. Simultaneous Optimistic Optimization (**SOO**)[1]
3. Infinite-Metric GP Optimization (**IMGPO**)[2]

Experimental results



- For all algorithms, the cells are divided into 3 smaller children along the longest dimension.
- SOO and IMGPO works in 7 dimensions with bound [0,1] for each dimension.
- For ML-SOO, the bound is initially set [-1,1] for the first and third cases and [-2,2] for the second case and the bound's width is reduced by p=4 every time new dimensions are added.

Conclusions

A novel extension of Simultaneous Optimistic Optimization (SOO) for infinite dimensional optimisation has been presented for the first time in this paper. The objective of the algorithm is to find a curve or a 1D function to obtain the maximum value of the given functional. The algorithm has been tested against the original SOO and IMGPO with fixed dimensions to solve analytically known physical systems, such as the brachistochrone and the catenary problems. In all test cases, the new multi-level SOO gives faster convergence to the actual solution, compared to the other two algorithm.

The biggest advantage of using multi-level SOO to optimise physical systems is that it does not need the gradient of the system, just a functional to calculate the value of tested functions. It is suitable to optimise shapes in physical systems that require simulations to compute the functional values.

References

[1] R. Munos, Optimistic Optimization of a Deterministic Function without the Knowledge of its Smoothness. In *NIPS*, 2011.
[2] K. Kawaguchi, L. P. Kaelbling, T. Lozano-Perez. Bayesian Optimization with Exponential Convergence. In *NIPS*, 2015.

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