
Infinite dimensional optimistic optimisation with applications on physical systems

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Abstract

This paper presents a novel numerical optimisation method for infinite dimensional optimisation. The functional optimisation makes minimal assumptions about the functional and without any specific knowledge on the derivative of the functional. The algorithm has been tested on several physical systems (brachistochrone and catenary problems) and it is shown that the solutions obtained are close to the actual solutions in one thousand functional evaluations. It is also shown that for the tested cases, the new algorithm provides better convergence to the optimum value compared to the tested existing algorithms.

1 Introduction

Bayesian optimisation (BO) [1, 2] is a powerful tool to optimise functions with some prior assumptions about the function. The common process in which BO is utilised is a Gaussian process (GP) [3]. In GP, points in the function to be optimised are assumed to be correlated with the points surrounding them. Several algorithms have been proposed using GP. Among them are GP Probability Improvement (GP-PI) [4], GP Expected Improvement (GP-EI) [5], and GP Upper Confidence Bound (GP-UCB) [6, 7]. In these algorithms, several samples of the functions are taken and then the posterior distribution of the function for the unseen positions is updated. The algorithms then compute a number of acquisition functions for every unseen position and take a sample from the position that gives the highest acquisition function. It has been shown theoretically that GP-UCB will eventually converge to the global maximum of a function, provided that the next sampled point is the point that has the highest upper confidence bound [6].

One major drawback of GP is that it needs an auxiliary search to look for the highest acquisition function value. Auxiliary search is hard and costly to perform in practice, especially when the number of dimensions is high. Simultaneous Optimistic Optimisation (SOO) [8] is an optimisation algorithm that does not need an auxiliary search. Several methods also take advantage of SOO and BO by combining them, such as in BaMSOO [9] and IMGPO [10]. However, these algorithms only work in a moderate number of dimensions and they do not perform well in higher dimensions.

In physical applications, there are several problems that require optimisation of functionals, instead of functions. Simple examples are “what is the trajectory of a ball to reach some points in the shortest amount of time?” (brachistochrone), and “what is the shape of a moving object to minimise the drag in a fluid?”. These problems can be simulated to calculate the functionals, but it is difficult to calculate the gradient of the functionals. As a result, the optimisation algorithm required is one that does not compute gradients and yet can still work for functionals. In this paper, an extension of SOO is presented to work for optimising functionals and it will be tested later to solve several physical problems.

2 Simultaneous Optimistic Optimisation (SOO)

Consider a function, $f : \mathcal{X} \rightarrow \mathbb{R}$ with $\mathcal{X} \subset \mathbb{R}^D$, a bounded set in \mathbb{R}^D . In most cases, \mathcal{X} is a hyper-rectangle with D dimensions. The function has at least a global optimiser, $x^* \in \mathcal{X}$ of f , and for all $x \in \mathcal{X}$, it is assumed that $f(x^*) - f(x) \leq l(x^*, x)$. The function $l : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a semi-metric function between two points in \mathcal{X} .

With the properties and assumptions above, R. Munos [8] advised optimistic optimisation algorithms to find the global optimum value of f . One of the algorithms, Simultaneous Optimistic Optimisation (SOO), does not even need to know the knowledge of the semi-metric function, l .

SOO is a tree-based search algorithm which partitions the search space, \mathcal{X} into several cells. Initially, there is only one cell, which contains all the search space. The central point of the cell is evaluated. This is the root of the tree. Then the cell is divided into K smaller cells and the centre points of the cells are evaluated. The smaller cells become the children of the divided cell. If a cell has a centre value larger than any cells with larger or the same size, then the cell is divided. The tree's depth is limited by a function of the number of evaluations, $h_{max}(n)$. The pseudo-code of the algorithm is shown in 1, where the i -th cell of depth h is denoted as (h, i) and the central value of the cell is $x_{h,i}$.

Algorithm 1 Simultaneous Optimistic Optimisation (SOO)

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 $\mathcal{T} \leftarrow (0, 0)$ ;  $n \leftarrow 0$ ; and  $\mathcal{L}_{\mathcal{T}} :=$  any nodes in  $\mathcal{T}$  without children
repeat
   $v_{max} \leftarrow 0$ 
  for  $h \leftarrow 0$  to  $\min(\text{depth}(\mathcal{T}), h_{max}(n))$  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  $x_n^+ \leftarrow \arg \max_{(h,i) \in \mathcal{T}} f(x_{h,i})$ 

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The regret of the algorithm after n function evaluations is defined as $r_n = f(x^*) - f(x_n^+)$, where $f(x_n^+)$ is the maximum value found so far. For some functions, the regret is even exponential, i.e. $r_n = \mathcal{O}(e^{-C\sqrt{n}/D})$ for some constant, C . SOO is also combined with Gaussian Processes to give better empirical performance and theoretical guarantee, as seen in BaMSOO [9] and IMGPO [10].

3 Multi-level SOO

SOO is a powerful algorithm to optimise function with moderate dimensions (e.g. 10 dimensions). However, to optimise functionals that have infinite dimensions, some modifications are required.

Suppose that we have a 1D function, $f : \mathcal{X} \rightarrow \mathcal{F}$ where $\mathcal{X}, \mathcal{F} \subset \mathbb{R}$, which is an input of a functional, $J : \mathcal{F}^{\mathcal{X}} \rightarrow \mathbb{R}$. The problem considered here is to find a function, f_* , to maximise the black-box functional, J , i.e. $f_* = \arg \max_{f \in \mathcal{F}^{\mathcal{X}}} J[f]$.

It is assumed that the end points of f are fixed, i.e. at $f(x_a)$ and $f(x_b)$, where $x_a < x_b$. The functional is also assumed to be Fréchet differentiable and f_* is twice differentiable. In order to solve it numerically, the function $f(x)$ is discretised at regular spacing points and then the number of discrete points in $f(x)$ is gradually increased. The values of $f(x)$ for $x \in \mathcal{X}$ is obtained by linearly interpolating the values from the discretised points.

Let one denote $f^{(l)}(x)$ as the discretised function of $f(x)$ at $2^l - 1$ points, excluding the end points, with spacing $h = (x_b - x_a)/2^l$, and then interpolate linearly. The number of discretised points will always be counted without the end points, unless indicated. The set of all possible discretised functions is denoted as $\mathcal{F}^{\mathcal{X}^{(l)}}$, where $\mathcal{F}^{\mathcal{X}^{(1)}} \subset \mathcal{F}^{\mathcal{X}^{(2)}} \subset \dots \subset \mathcal{F}^{\mathcal{X}}$. The discretised optimiser function, f_* , is denoted by $f_*^{(l)}(x)$. The global optimiser in $\mathcal{F}^{\mathcal{X}^{(l)}}$ is defined as $f_+^{(l)}(x) = \arg \max_{f \in \mathcal{F}^{\mathcal{X}^{(l)}}} J[f]$. The global optimiser in $\mathcal{F}^{\mathcal{X}^{(l)}}$ is not necessarily the same as $f_*^{(l)}$, but $f_+^{(l)} \rightarrow f_*^{(l)}$ as $l \rightarrow \infty$.

Assumption 1 For a Fréchet differentiable functional, $J[f]$, there exists $L > 0$ and $\eta \in (0, 1)$ where $\eta L \|f_* - f\|_1^2 \leq J[f_*] - J[f] \leq L \|f_* - f\|_1^2$ for all $f \in \mathcal{F}^X$.

Lemma 2 The L_1 -distance between $f_+^{(l)}$ and f_* is bounded by $\|f_* - f_+^{(l)}\|_1 \leq \alpha 4^{-l}$ for some α .

The variable α depends on the intrinsic parameters of J and f_* . From the lemma above, the search space can be decreased by 4^{-l} as l increased, provided α is chosen to be large enough. Based on lemma 2, it is possible to perform optimisations using SOO as in Algorithm 1 with the use of several rules in dividing cells as below, letting $p = 4$.

(1) The initial cell is one dimensional with a width of w and $l = 1$. The position of the central point of the cell represents the value of a point in $x = (x_a + x_b)/2$. **(2)** If all dimensions in the cell have lengths less than or equal to p^{-l} , then new 2^l dimensions are added to the cell. The new dimensions represent the position of the new points in the discretised $f^{(l+1)}(x)$ which is placed in the middle positions of discretised points in $f^{(l)}(x)$. The new dimensions have widths of p^{-l} each. The value of l is also increased by 1. **(3)** A cell is divided along the longest dimension into $K = 3$ smaller cells as in [10]. If there are more than one dimension that have the same length, then the ‘oldest’ dimension is chosen. **(4)** If a cell is divided along an ‘old’ dimension, the change in position in the dimension will also change the position in the ‘newer’ dimensions around it.

As an example let $p = K = 3$. The first cell has $l = 1$ and only specifies $D = 2^l - 1 = 1$ points on f , which is $x_1^{(1)}$, the middle point between x_a and x_b . On the first division, the cell is divided into 3 smaller cells along the first dimension. After the division, the children’s dimension width is now 3^{-1} and it is equal to p^{-l} with $p = 3$ and $l = 1$. Therefore, $2^l = 2$ new dimensions are added to the children cell which correspond to the middle points between x_a and $x_1^{(1)}$, and between $x_1^{(1)}$ and x_b .

With $l = 2$ and $D = 2^l - 1 = 3$ dimensions, let one denote the discretised points as $x_i^{(2)}$ with $i \in \{1, 2, 3\}$. The second dimension is the oldest dimension because it was the same dimension as the dimension with $l = 1$. The first and third dimensions are the newer dimensions. As all the dimensions now has width of 3^{-1} , the older dimension is divided first, i.e. $i = 2$. Because an older dimension is divided, some of its children have different positions in the second dimension and thus change the positions in the first and third dimensions. If one of the children is shifted in the second dimension by $\Delta x_2^{(2)}$ with respect to its parent’s position, then the first and third dimensions also shift by $\Delta x_2^{(2)}/2$, because linear interpolation is used.

For the next division, as the longest dimensions are the first and the third dimension, it can choose any dimension to be divided. As the divided dimension is the newest dimension, it does not shift the positions in other dimensions. The division process of cells is repeated until the algorithm stops.

One can use different methods of interpolation other than linear interpolation. If a different method is used, it changes the upper limit of p , but it also needs different assumptions on the optimal function, f_* . For example, quadratic interpolation yields the upper limit of p to be 16, but the fourth derivative of f_* needs to be bounded. Increasing the order of polynomial in the interpolation does not always help, because the upper bound of m -th derivative of f_* can increase as in Runge’s phenomenon [11].

4 Numerical Experiments

To test the performance of the algorithm, some numerical experiments on physical cases have been performed. The algorithm is benchmarked against SOO [8] and IMGPO [10]. Those algorithms are also gradient-free optimisations. As the other algorithms are designed for fixed dimensions search space, it is tested with $D = 7$ dimensions.

The algorithms are tested for solving brachistochrone and catenary problems. The first case is brachistochrone problem, where the algorithms need to determine the path between 2 points in 2D space so that an object starting from the first point can travel in influence of gravity to the other point as fast as possible. The gravity is assumed to be 1. The positions of the end points are $(0, 0)$ and $(1, 0)$ and the beads have initial velocity $v_0 = \sqrt{2/(2 + \pi)}$. The minimum time required in this case is $\pi/\sqrt{2 + \pi}$. The second case is catenary problem, which is the minimum area when the path between two end points is rotated along the x -axis. The end points are located at $(0, 0)$ and $(1, 0)$. The third case is brachistochrone problem with linear drag, $F_d = -\beta v$ with $\beta = 0.02$. The end points are

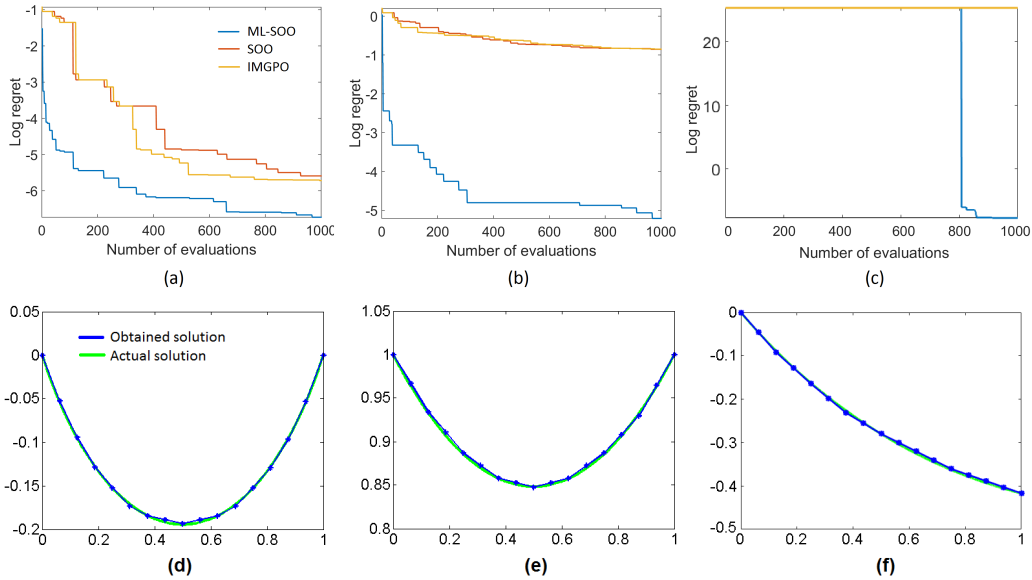


Figure 1: Top: Log regret versus number of functional evaluations using multi-level SOO, SOO, and IMGPO for (a) the brachistochrone problem, (b) the catenary problem, and (c) the brachistochrone problem with drag. Bottom: Comparison of the solutions obtained by the algorithm with the actual solutions. In the third case, SOO and IMGPO do not find a possible solution to travel to the other end.

located at $(0, 0)$ and $(1, 0.417)$. The object has initial velocity of $v_0 = 1.19$. The brachistochrone with drag is a complicated problem where the solution and Fréchet derivative cannot be obtained in a straightforward manner. The actual solutions for the test cases are cycloid, hyperbolic cosine, and the equation (35) from [12], respectively. Output of the functional is the negative value of time required to travel such shape. It returns a very large number if it is impossible to reach the other end.

In SOO and IMGPO, a cell is divided into three smaller children along the longest dimension. The parameters that were used in IMGPO are the parameters used in [10]. The search space for the algorithms is confined to $[0, 1]$ for each dimension. For the new algorithm, the initial bound is set to be $[-1, 1]$, except in the second case where the bound is $[-2, 2]$. The bound is reduced by factor of 4 every time new dimensions are added.

The performance of the algorithms in all test cases is shown in Figure 1(a)-(c). The solutions obtained by the new algorithm are also plotted with the optimum solution in Figure 1(d)-(f). As demonstrated in the figures, the new algorithm performs better than the other algorithms in all test cases. The solutions obtained by the new algorithm are also quite close to the optimum solutions. In all cases, the solution found by the new algorithm consists of 15 points which is already more than the dimensions tested by other algorithms. The number of discretised points in the solutions can be increased by running the algorithm for longer.

5 Conclusion

A novel extension of Simultaneous Optimistic Optimisation (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 algorithms.

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.

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