Derivative-free Efficient Global Optimization on High-dimensional Simplex

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Abstract In this paper, we develop a novel derivative-free deterministic greedy algorithm for global optimization of any objective function of parameters belonging to a unit-simplex. Main principle of the proposed algorithm is making jumps of varying step-sizes within the simplex parameter space and searching for the best direction to move in a greedy manner. Unlike most of the other existing methods of constraint optimization, here the objective function is evaluated at independent directions within an iteration. Thus incorporation of parallel computing makes it even faster. Requirement of parallelization grows only in the order of the dimension of the parameter space, which makes it more convenient for solving high-dimensional optimization problems in simplex parameter space using parallel computing. A comparative study of the performances of this algorithm and other existing algorithms have been shown for some moderate and high-dimensional optimization problems along with some transformed benchmark test-functions on simplex. Around 20 – 300 folds improvement in computation time has been achieved using the proposed algorithm over Genetic algorithm with more accurate solution.

Keywords Simplex · coordinate descent · gradient descent · convex optimization · non-convex global optimization · Genetic algorithm

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1 Introduction

$k$-simplex is defined as a $k$-dimensional polytope, which is a convex hull of its $k + 1$ affinely independent vertices. Consider $\{v_1, \ldots, v_m\} \in \mathbb{R}^{m-1}$ are $m$ affinely independent vertices of the convex-hull $\mathbb{H}$ in $\mathbb{R}^{m-1}$. Then all points in $\mathbb{H}$ can be described by the set

$$S_H = \{p_1v_1 + \cdots + p_mv_m | p_i \geq 0, 1 \leq i \leq m, \sum_{i=1}^{m} p_i = 1\}$$

Clearly, $S_H$ is a $(m-1)$-dimensional simplex. Consider a case where an objective function has to be optimized on the parameter space is given by $\mathbb{H}$. For any point $v \in \mathbb{H}$, we would get an unique $m$-tuple $p = (p_1, \cdots, p_m)$ such that $p_i \geq 0$ for $i = 1, \ldots, m$ and $\sum_{i=1}^{m} p_i = 1$. Thus, we can write our objective function as a function of $p = (p_1, \cdots, p_m)$. So our problem can be formulated as

$$\begin{align*}
\text{minimize} & : f(p_1, \cdots, p_m) \\
\text{subject to} & : p_i \geq 0, 1 \leq i \leq m, \sum_{i=1}^{m} p_i = 1. 
\end{align*}$$

(1)

In the field of computational mathematics, statistics and operational research, optimization problems on the simplex parameter space are pretty common. For example, some of the useful and convenient methods like modeling with splines (specifically B-splines), estimation problem in multinomial setup, Markov chain transition matrix estimation and estimation of mixture proportions of mixture distribution are a few of them. But there is a scarcity of specially designed algorithms for non-linear optimization of parameters coming from simplex.

There exist many algorithms for optimizing linear functions on constrained linear space as well as on simplex. For non-linear objective functions, convex optimization algorithms can be used when the objective function is also convex. ‘Interior-point (IP)’ algorithm (see [5], [6], [7], [8]) and ‘Sequential Quadratic Programming (SQP)’ algorithm (see [9], [8], [10]) are widely used for non-linear convex optimization problems. The simplex parameter space being convex, IP and SQP algorithms can be used for convex optimization for optimization of objective functions where parameters are in simplex. Although, the main problem with these convex optimization algorithms is that it gets stuck at any local minima in case the objective function is non-convex with multiple minimas. One possible solution to avoid this problem is starting the iterations from several starting points. Although, for low dimensional non-convex optimization problems, the strategy of starting from multiple initial points might be affordable. But with increasing dimension of the parameter space, this strategy proves to be computationally very expensive since with increasing dimension, the requirement of number of starting points increase exponentially. So, it is of interest to find an efficient algorithm for non-convex
optimization on simplex constrained space.

In the last few decades, many non-convex global optimization strategies have been proposed on constrained spaces. The ‘Genetic algorithm (GA)’ (see [12], [13], [14]) and ‘Simulated annealing (SA)’ (see [15], [16]) remained quite popular among them. GA works fine for lower dimensional problems. But GA does not scale well with complexity because in higher dimensional optimization problems there is often an exponential increase in search space size (see [17], page 21). Besides, one major problem with these two methods is they might be much expensive in case we use these methods for simple convex functions.

With the increasing access to high-performance modern computers and clusters ([21]), some of the existing parallelizable optimization algorithms (e.g., Monte Carlo methods) have a great advantage for certain types of problems. The motivation behind using parallelization in these methods is mainly to either start from different starting points or to use different random number generator seeds simultaneously. As mentioned earlier, though these methods perform well for lower dimensional parameter spaces, since with an increasing number of dimensions, parameter space grows exponentially, the way these methods use parallelization, is not much helpful. On the other hand, parallelization can only increase the sampling rates linearly. Instead, if we can design an algorithm where requirement of parallelization increases linearly with the dimension of the parameter space, it would be more convenient and useful for high-dimensional parameter spaces on simplex.

The main principle of our algorithm is to make jumps along the coordinates of the parameter of varying step sizes within the parameter space and search for the best possible direction of movement in a greedy manner during each iteration step. In most of the existing methods, during an update stage, it finds out the best possible direction of the movement (in terms of the objective function values at those sites) by derivative based methods (e.g., ‘interior point’ and ‘SQP algorithms). Though derivative based methods work quite fast and well enough for smooth objective functions, but for all objective functions, there might not exist a closed form of the derivative. In that case, numerical evaluation of derivative might affect the computational efficiency. Secondly, relying on derivative based methods, there is always a chance of converging to local extrema. The strategy of choosing a parameter randomly and moving with step size (may be adaptive) depending on it’s effect on the objective function works well for low-dimensional problems. But with increasing number of parameters, at every iteration, it is important to move in the direction which has the minimum value of the objective function. In a high-dimensional optimization problem, choosing the parameters’ axes randomly for updates (e.g., [18]) decreases the chance of the moving in the best possible direction during iterations. This motivates us to find a novel way for selecting the best possible direction of movement during each iteration step instead of
randomly choosing any parameter axis or direction.

To avoid derivative, we can moving along the co-ordinates of the parameter with varying step-sizes and choose the best possible direction of movement. In our algorithm during an iteration, once we fix the step size (say $s$), for any co-ordinate of the parameter, there are two available options for movement, either increase or decrease by that step size $s$. For $m$-dimensional parameter space, the step-size, by which a co-ordinate position of the parameter is increased, is deducted from the rest of the co-ordinates of the parameter equally to maintain the constraint $\sum_{i=1}^{m} p_i = 1$. For example, if we increase the first co-ordinate by step size $s$ at a step, we subtract $s/(m-1)$ from rest of the co-ordinates $i = 2, \ldots, m$ of the parameters. Hence for a given step size, there are $2m$ possible directions of movement since we are moving only one co-ordinate position of the parameter at a time by that step-size $s$ in positive and negative directions and the corresponding constraint adjustment is done as mentioned above (discussion on how to account for boundary issues and how to determine and vary step sizes has been mentioned in Section 2). Thus during each iteration, we find $2m$ possible movements in the neighborhood of the current parameter value. After checking the objective function value at those $2m$ possible directions of movement, the direction of movement where the objective function has the minimum value is chosen and compared with the value of the objective function at the current site (before making any movements). New updated value of the parameter is set equal to the site with lower objective function value among those two aforementioned sites. Thus the best possible direction of movement in the neighborhood of the current value of the parameter is ensured at each iteration. Another advantageous side of our algorithm is that we can evaluate the objective function at possible $2m$ directions in parallel. Thus the requirement of parallel computing only increases in the order of the number of parameters, unlike the way Monte Carlo uses parallel computing as mentioned above. We call this algorithm ‘Greedy Coordinate Descent of Varying Step-size on Simplex’ (GCDVSS).

2 Algorithm

Suppose we have a objective function $Y = f(p)$ where $p = (p_1, \ldots, p_m)$ is a vector of length $m$, such that, $\sum_{i=1}^{m} p_i = 1$ and $p_i \geq 0$ for $i = 1, \ldots, m$. Our objective is

$$\text{minimize } : f(p_0, p_1, \ldots, p_m)$$

$$\text{subject to } : p_i \geq 0, \ 0 \leq i \leq m, \ \sum_{i=0}^{m} p_i = 1. \quad (2)$$
Define
\[ S = \{ p = (p_1, \ldots, p_m) \in \mathbb{R}^m \mid \sum_{i=1}^{m} p_i = 1, p_i \geq 0, 0 \leq i \leq m \} \]

Our problem can be written as
\[
\begin{align*}
\text{minimize} & : f(p) \\
\text{subject to} & : p \in S
\end{align*}
\]

Our algorithm consists of several runs. Each run is an iterative procedure. A run stops based on some convergence criteria (see below). At the end of each run, a solution is returned. For the first run only, the starting point should be provided by the user. But for the following runs, it starts from the solution returned by the previous run. Each run tries to minimize the objective function value in a greedy manner (see below for details). Hence, the solution gets improved after each run. Once two consecutive runs yield the same solution, our algorithm stops returning the final solution.

In our algorithm, each run is a similar iterative procedure except the fact that the values of tuning parameters after each run might be changed. In each run there are four tuning parameters which are initial global step size \(s_{\text{initial}}\), step decay rate \(\rho\), step size threshold \(\phi\) and sparsity threshold \(\lambda\). Except step decay rate \(\rho\), the values of the other tuning parameters are fixed at the beginning and kept unchanged till the algorithm converges. The value of step decay rate is taken to be \(\rho = \rho_1\) for the first run and \(\rho = \rho_2\) for the following runs. Overall there are 5 tuning parameters which are \(s_{\text{initial}}, \rho_1, \rho_2, \phi\) and \(\lambda\). Apart from these parameters, \(\text{max\_iter}\) denotes the maximum number of allowed iterations inside a run. \(\text{max\_runs}\) denotes the maximum number of allowed runs.

Inside each run, there is a parameter called global step size and 2m local parameters named local step sizes (denoted by \(s_i^+\) and \(s_i^-\)). In the first iteration of each run, we set initial value of global step size \(s^{(1)} = s_{\text{initial}}\). It’s value is kept unchanged throughout a iteration. But at the end of each iteration, it’s value is either kept same or decreased by a division factor step decay rate \(\rho\), based on some convergence criteria (see below, see step (7) of STAGE 1). Hence, in the \((j+1)\)-th iteration, the global step size is \(s^{(j+1)}\) would be equal to \(s^{(j)}\) or \(\frac{s^{(j)}}{\rho}\) based on the aforementioned criteria. At the beginning of any iteration, the local step sizes are set equal to the current global step size. For example, at the beginning of \(j\)-th iteration, we set \(s_i^+ = s_i^- = s^{(j)}\) for \(i = 1, \ldots, m\). Suppose the current value of \(p\) in the \(j\)-th iteration is \(p^{(j)} = (p_1^{(j)}, \ldots, p_m^{(j)}) \in S\). During the \(j\)-th iteration, we look for 2m points within the domain \(S\) which can be reached by moving from the current solution \(p^{(j)}\) and the movements depend on the local step sizes. The value of the local step sizes are subject to be updated if the movements corresponding to those step sizes yield points in \(\mathbb{R}^m\) outside \(S\) (see step (3) and (4) of STAGE
1). Note that, once the value of a co-ordinate goes below the sparsity threshold \( \lambda \), we consider those co-ordinates to be ‘insignificant’. Suppose \( l \)-th component of \( p^{(j)} \) is ‘insignificant’. Then for the evaluations of \( q^+ \) and \( q^- \) for \( i \neq l \), \( p^{(j)}_i \) is kept unchanged (see step (3) and (4) of STAGE 1). If the points \( q^+ \) and \( q^- \) for \( i = 1, \ldots, m \) are in \( S \), the values of the objective function are evaluated at those points and are saved as \( \{ f^+_i \}_{i=1}^m \) and \( \{ f^-_i \}_{i=1}^m \) for \( i = 1, \ldots, m \).

Once \( \{ f^+_i \}_{i=1}^m \) and \( \{ f^-_i \}_{i=1}^m \) are evaluated for \( j \)-th iteration, we find the smallest one out of these \( 2m \) values. If the smallest of these \( 2m \) values is smaller than \( f(p^{(j)}) \), the point corresponding to that smallest value of the objective function is accepted. Then the ‘insignificant’ positions are replaced by 0 and the sum of the ‘insignificant’ positions (named ‘garbage’) is divided by the number of remaining positions and that derived quantity is added to those remaining positions. After that, this new point is considered as the updated \( p^{(j)} \) and the value of \( p^{(j+1)} \) is set equal to that obtained point (see step (5) and (6) of STAGE 1). Once the square of the euclidean distance of the objective function parameters of two consecutive iterations becomes less than \( tol_{\text{fun}} \), the global step size is decreased by a division factor of \( \rho \), the step decay rate (see step (7) of STAGE 1). A run ends when the global step size becomes less than or equal to step size threshold \( \phi \) (see step (8) of STAGE 1). Once same solution is returned by two consecutive runs, our algorithm stops after returning the final solution.

The default value of \( s_{\text{initial}} \) is taken to be equal to 1. \( \rho_1 \) and \( \rho_2 \) denote the step decay rates. Taking smaller step decay rate results in better solution in the cost of higher computation time. Based on experiments, we note that we get satisfactory results for setting the default values of these parameters \( \rho_1 = 2 \) and \( \rho_2 = 1.05 \). \( \phi \) denotes minimum allowed size of the global step size for movement within the domain (see the algorithm for dependence of the movement of the global step size). Making the value of \( \phi \) smaller results into more accurate solution in the cost of higher computation time. It’s default value is taken to be equal to \( 10^{-3} \). \( \lambda \) controls the sparsity. At the end of each iteration, the positions of the current estimated parameter with values less than \( \lambda \) are set equal to 0 (see step (6) of STAGE 1). Also, \( \lambda \) controls the movement of the parameters of the objective function in the domain (see step (3) and (4) of STAGE 1). In case, the solution is expected to be sparse, it’s value should be set larger and in case, the solution is not expected to be sparse, it’s value should be set smaller. We note, in general, the default value of \( \lambda = 10^{-3} \) works fine. We set \( \text{max.iter} = 50000, \text{max.runs} = 1000 \) and \( tol_{\text{fun}} = 10^{-15} \). Before going through the STAGE 1 for the first time, we set \( R = 1, \rho = \rho_1 \) and initial guess of the solution \( p^{(1)} = (p^{(1)}_1, \ldots, p^{(1)}_m) \in S \).

**STAGE : 1**

1. Set \( j = 1 \). Set \( s^{(j)} = s_{\text{initial}} \) Go to step (2).
2. If $j > \text{max}\_\text{iter}$, set $\hat{p} = p^{(j-1)}$. Go to step (9). Else, set $s_i^+ = s_i^- = s^{(j)}$ and $f_i^+ = f_i^- = Y^{(j)} = f(p^{(j)})$ for all $i = 1, \ldots, m$. Set $i = 1$ and go to step (3).

3. If $i > m$, set $i = 1$ and go to step (4). Else, find $K_i^+ = n(S_i^+)$ where $S_i^+ = \{l \mid p_i^{(j)} > \lambda, l \neq i\}$. If $K_i^+ \geq 1$, go to step (3.1), else set $i = i + 1$ and go to step (3).

(a) If $s_i^+ \leq \phi$, set $i = i + 1$ and go to step (3). Else (if $s_i^+ > \phi$), evaluate vector $q_i^+ = (q_{i1}^+, \ldots, q_{im}^+)$ such that

$$q_{il}^+ = p_i^{(l)} + s_i^+ \text{ for } l = i$$

$$= p_i^{(l)} - \frac{s_i^+}{K_i^-} \text{ if } l \in S_i^-$$

$$= p_i^{(l)} \text{ if } l \in (S_i^+ \cup \{i\})^C$$

Go to step (3.2).

(b) Check whether $q_i^+ \in S$ or not. If $q_i^+ \in S$, go to step (3.3). Else, set $s_i^+ = \frac{s_i^+}{p}$ and go to step (3.1)

(c) Evaluate $f_i^+ = f(q_i^+)$. Set $i = i + 1$ and go to step (3).

4. If $i > m$, go to step (5). Else, find $K_i^- = n(S_i^-)$ where $S_i^- = \{l \mid p_i^{(j)} > \lambda, l \neq i\}$. If $K_i^- \geq 1$, go to step (4.1), else set $i = i + 1$ go to step (4).

(a) If $s_i^- \leq \phi$, set $i = i + 1$ and go to step (4). Else (if $s_i^- > \phi$), evaluate vector $q_i^- = (q_{i1}^-, \ldots, q_{im}^-)$ such that

$$q_{il}^- = p_i^{(l)} - s_i^- \text{ for } l = i$$

$$= p_i^{(l)} + \frac{s_i^-}{K_i^-} \text{ if } l \in S_i^-$$

$$= p_i^{(l)} \text{ if } l \in (S_i^- \cup \{i\})^C$$

Go to step (4.2)

(b) Check whether $q_i^- \in S$ or not. If $q_i^- \in S$, go to step (4.3). Else, set $s_i^- = \frac{s_i^-}{p}$ and go to step (4.1)

(c) Evaluate $f_i^- = f(q_i^-)$. Set $i = i + 1$ and go to step (4).

5. Set $k_1 = \arg\min_{1 \leq l \leq m} f_i^+$ and $k_2 = \arg\min_{1 \leq l \leq m} f_i^-$. If $\min(f_{k1}^+, f_{k2}^-) < Y^{(j)}$, go to step (5.1). Else, set $p^{(j+1)} = p^{(j)}$ and $Y^{(j+1)} = Y^{(j)}$, set $j = j + 1$. Go to step (7).

(a) If $f_{k1}^+ < f_{k2}^-$, set $p_{\text{temp}} = q_{k1}^+$, else (if $f_{k1}^+ \geq f_{k2}^-$), set $p_{\text{temp}} = q_{k2}^-$. Go to step (6).

6. Find $K_{\text{updated}} = n(S_{\text{updated}})$ where $S_{\text{updated}} = \{l \mid p_{\text{temp}}(l) > \lambda, l = 1, \ldots, m\}$. Go to step (6.1).

(a) If $K_{\text{updated}} = m$, set $p^{(j+1)} = p_{\text{temp}}$, set $j = j + 1$. Go to step (7). Else, go to step (6.2).
(b) Set garbage = \( \sum_{j \in S_{\text{updated}}} p_{\text{temp}}(k) \).

\[
    p^{(j+1)}(l) = \begin{cases} 
        p_{\text{temp}}(l) + \text{garbage}/K_{\text{updated}} & \text{if } l \in S_{\text{updated}} \\
        0 & \text{if } l \notin S_{\text{updated}}
    \end{cases}
\]

Set \( j = j + 1 \). Go to step (7).

7. If \( \sum_{i=1}^{m} (p^{(j)}(i) - p^{(j-1)}(i))^2 < \text{tol} \cdot \text{fun} \), set \( s^{(j)} = s^{(j-1)}/\rho \). Go to step (8).

Else, set \( s^{(j)} = s^{(j-1)} \). Go to step (2).

8. STOP execution. Set \( z(R) = \tilde{p} \). Set \( R = R + 1 \). Go to STAGE 2.

STAGE : 2

1. If \( R \leq \text{max \_ runs} \) and \( z(R) \neq z(R-1) \), go to step (2). Else \( z(R) \) is the final solution. STOP and EXIT.

2. Set \( \rho = \rho_2 \) keeping other tuning parameters (\( \phi, \lambda \) and \( s_{\text{initial}} \)) fixed. Repeat algorithm described in STAGE 1 setting \( p^{(1)} = z(R) \).

At the end of each run, under certain set of assumptions and regularity conditions, our algorithm returns a local minima as the solution (see Section [4]). After first run, the following runs try to improve the solution returned by the previous run by making jumps of various step sizes in the parameter space and checking the objective function values at those sites. Thus, it tries to find a better solution even after reaching a local minima.

3 Order of Algorithm

In this section, we find the order of our algorithm both in terms of the number of basic operations required and the number of objective function evaluations required as functions of the dimension of the parameter space. Since we are trying to find the order of our algorithm, finding the upper bound of number of operations for worst case scenario would be sufficient to determine the order.

Suppose we want to minimize \( f(p) \) where \( p \in \mathbf{S} \). At the beginning of each iteration, 4 arrays of length \( m \), i.e., \( s^+, s^-, f^+, f^- \) are initialized (see step (2) of STAGE 1 in Section [2]). During each iteration, starting from the current value of the parameter \( 2m \) possible movements are looked for in a way such that each of them belongs to the domain \( \mathbf{S} \). Search algorithm for first \( m \) of these movements have been described in step (3) of STAGE 1 of Section [2].

Consider the search procedure for any one of these \( m \) movements. In the aforementioned step, note that it requires not more than \( m \) operations to find \( S^{+} \). To find \( K^{+} \), it takes at most \( m \) operations. As we are considering the worst case scenario in terms of maximizing the number of required operations, assume \( K^{+} \geq 1 \). In step (3.1) and (3.2) of STAGE 1, suppose the value of \( s^{+} \) is updated atmost \( k \) times. So, we have \( \frac{s^+_{\text{initial}}}{\rho^k} \leq \phi \) but \( \frac{s^+_{\text{initial}}}{\rho^k} > \phi \).
Hence \( k = 1 + \left\lceil \frac{\log \left( \frac{s_{\text{initial}} \phi}{\rho} \right)}{\log(p)} \right\rceil \), where \( \lceil x \rceil \) returns the largest integer less than or equal to \( x \). Corresponding to each update step of \( s_i^+ \), first it is checked whether \( s_i^+ \leq \phi \) or not. It involves a single operation. Then deriving \( q_{i+1} \) involves not more than \( 2m \) steps because the most complicated scenario occurs for updating the positions of \( q_{i+1} \) which belong to \( S_i^+ \). And in that case, it takes total two operations for each site, one operation to find \( s_i^+ \) and one more to evaluate to subtract that quantity from \( p_{(l)} \) for \( l \in S_i^+ \). After that, to check whether \( q_i \in S \) or not, it requires \( m \) operations. For the worst case scenario, we also add one more step required for updating \( s_i^+ = \frac{\phi}{\rho} \). Hence the search procedure of any movement (i.e., for any \( i \in \{1, \ldots, m\} \)) in step (3) of STAGE 1 requires \( m + m + k \times (1 + 2m + m + 1) = m \times (2 + 3k) + 2k \) operations. Hence, for \( m \) movements (mentioned in step (3) of STAGE 1 in Section 2) it requires not more than \( m^2 \times (2 + 3k) + 2mk \) operations. In a similar way, it can be shown that for step (4) also the maximum number of required operations is not more than \( m^2 \times (2 + 3k) + 2mk \).

In step (5) of STAGE 1 in Section 2, to find \( k_1 \) or \( k_2 \), it takes \((m - 1)\) operations. The required number of steps for this step will be maximized if \( \min(f_{k_1}, f_{k_2}) < Y^{(j)} \). Under this scenario, two more operations (i.e., comparisons) are required to find \( p_{\text{temp}} \). So this step requires not more than \( 2 \times (m - 1) + 2 = 2m \) operations.

In step (6) of STAGE 1 in Section 2 it takes at most \( m \) operations to find \( S_{\text{updated}} \). In case \( K_{\text{updated}} \) is not \( m \), the required number of operations spent in this step will be more than the case when \( K_{\text{updated}} = m \). For finding out the number of operations required for the worst case scenario, assume \( K_{\text{updated}} < m \). To find the value of \( \text{garbage} \), maximum number of required steps is not more than \( m \). Finally, it can be noted that in step (6.2), updating the value of the parameter of interest from \( p_{(j)} \) to \( p_{(j+1)} \) requires not more than \( 2m \) steps. So maximum number of operations required for step (6) of STAGE 1 is not more than \( m + m + 2m = 4m \).

In step (7) of STAGE 1 in Section 2, to find \( (p_{(j)}(i) - p_{(j-1)}(i))^2 \) for each \( i \in \{1, \ldots, m\} \), we need one operation for taking difference, and one operation for taking the square. Hence to find the sum of the squares, it needs \((m - 1)\) more operations. Comparing it’s value with \( \text{tol}_{\text{fun}} \) takes one more operation. In the worst case scenario, it would take two more operations till the end of the iteration, i.e., update of \( s^{(j)} \) at step (7) and it’s comparison with \( \phi \) at step (8). Hence after step (6), the required number of operations would be at most \((3m - 1) + 1 + 2 = 3m + 2 \).

Hence for each iteration, in the worst case scenario, the number of required basic operations is not more than \( m^2(2 + 3k) + 2mk + 2m + 3m + (3m + 2) = m^2(2 + 3k) + m(2k + 8) + 2 \). So, number of basic operations required for each
Hence there exist a \( N \) such that all its coordinates are positive. Define \( u \) from 1. Define coordinate can be derived by subtracting the sum of the first (\( r \) 1. Suppose \( u \) is a point in \( S \) such that all its coordinates are positive. Define \( u_k^{(+)} = (u_1 - \frac{\delta_k}{n-1}, \ldots, u_{i-1} - \frac{\delta_k}{n-1}, u_i + \delta_k, u_{i+1} - \frac{\delta_k}{n-1}, \ldots, u_n - \frac{\delta_k}{n-1}) \) and \( u_k^{(-)} = (u_1 + \frac{\delta_k}{n-1}, \ldots, u_{i-1} + \frac{\delta_k}{n-1}, u_i - \delta_k, u_{i+1} + \frac{\delta_k}{n-1}, \ldots, u_n + \frac{\delta_k}{n-1}) \) for \( i = 1, \ldots, n \). If for all \( k \in N \), \( f(u) \leq f(u_k^{(+)}) \) and \( f(u) \leq f(u_k^{(-)}) \) (whenever \( u_k^{(+)}, u_k^{(-)} \in S \)) for all \( i = 1, \ldots, n \), the global minimum of \( f \) occurs at \( u \).

**Proof (Proof of Theorem)** Fix some \( i \in \{1, \ldots, n\} \). Define
\[
\begin{align*}
  r_1 &= \min\{(n-1)u_1, \ldots, (n-1)u_{i-1}, (1-u_1), (n-1)u_{i+1}, \ldots, (n-1)u_n\}, \\
  r_2 &= \min\{(n-1)(1-u_1), \ldots, (n-1)(1-u_{i-1}), u_1, (n-1)(1-u_{i+1}), \ldots, (n-1)(1-u_n)\}
\end{align*}
\]
Set \( r = \min\{r_1, r_2\} \). Since \( \delta_k \) is strictly decreasing sequence going to zero, there exist a \( n \in \mathbb{Z} \) such that for all \( k \geq N \), \( \delta_k < r \). Fix some \( i \in \{1, \ldots, n\} \). Hence \( u_N^{(+)}, u_N^{(-)} \in S \).

Once we fix the first \( (n-1) \) coordinates of any element in \( S \), the \( n \)-th coordinate can be derived by subtracting the sum of the first \( (n-1) \) coordinates from 1. Define
\[
S^* = \{(x_1, \ldots, x_{n-1}) \in \mathbb{R}^{n-1} : \sum_{i=1}^{n} x_i < 1, x_i \geq 0, i = 1, \ldots, n-1\}.
\]
Define \( u^* = (u_1, \ldots, u_{n-1}) \) and
\[
\begin{align*}
  u_k^{(+) &= (u_1 - \frac{\delta_k}{n-1}, \ldots, u_{i-1} - \frac{\delta_k}{n-1}, u_i + \delta_k, u_{i+1} - \frac{\delta_k}{n-1}, \ldots, u_{n-1} - \frac{\delta_k}{n-1})} \\
  u_k^{(-) &= (u_1 + \frac{\delta_k}{n-1}, \ldots, u_{i-1} + \frac{\delta_k}{n-1}, u_i - \delta_k, u_{i+1} + \frac{\delta_k}{n-1}, \ldots, u_{n-1} + \frac{\delta_k}{n-1})}
\end{align*}
\]
for \( i = 1, \ldots, n - 1 \). Note that \( \mathbf{u}^*, \mathbf{u}_k^{(i+)} \), \( \mathbf{u}_k^{(i-)} \) are the first \((n - 1)\) coordinates of \( \mathbf{u}, \mathbf{u}_k^{(i+)} \), \( \mathbf{u}_k^{(i-)} \) respectively. Define \( f^*: S^* \mapsto \mathbb{R} \) such that

\[
f^*(x_1, \ldots, x_{n-1}) = f(x_1, \ldots, x_{n-1}, 1 - \sum_{i=1}^{n-1} x_i).
\]

Hence we have \( f^*(\mathbf{u}^*) = f(\mathbf{u}), \ f^*(\mathbf{u}_k^{(i+)}') = f(\mathbf{u}_k^{(i+)}) \) and \( f^*(\mathbf{u}_k^{(i-)}') = f(\mathbf{u}_k^{(i-)}) \). Since, \( f \) is continuous and differentiable on \( S \), \( f^* \) is continuous and differentiable on \( S^* \). Convexity of \( f \) implies \( f^* \) is convex on \( S^* \). Consider \( x_1^*, x_2^* \in S^* \). Suppose \( x_1, x_2 \in S \) are such that their first \((m - 1)\) co-ordinates are same as \( x_1^* \) and \( x_2^* \) respectively. Take any \( \gamma \in (0, 1) \). Now

\[
\gamma f^*(x_1^*) + (1 - \gamma) f^*(x_2^*) = \gamma f(x_1) + (1 - \gamma) f(x_2)
\]

\[
\geq f(\gamma x_1 + (1 - \gamma)x_2)
\]

\[
= f^*(\gamma x_1^* + (1 - \gamma)x_2^*).
\]

Hence \( f^* \) is also convex. Define \( h_i: U_i \mapsto S^* \) such that

\[
h_i(z) = (u_1 - \frac{z}{n - 1}, \ldots, u_{i-1} - \frac{z}{n - 1}, u_i + z, u_{i+1} - \frac{z}{n - 1}, \ldots, u_{n-1} - \frac{z}{n - 1})
\]

for \( i = 1, \ldots, n - 1 \), where \( U_i = [-\delta_N, \delta_N] \) (since each co-ordinate of \( \mathbf{u} \) is positive, \( \mathbf{u}^* \in S^* \). Note that the way \( N \) is chosen ensures \( h_i(U_i) \subset S^* \). Define \( g_i: U_i \mapsto \mathbb{R} \) for \( i = 1, \ldots, n - 1 \) such that \( g_i = f^* \circ h_i \). Hence we have

\[
g_i(z) = f^*(u_1 - \frac{z}{n - 1}, \ldots, u_{i-1} - \frac{z}{n - 1}, u_i + z, u_{i+1} - \frac{z}{n - 1}, \ldots, u_{n-1} - \frac{z}{n - 1})
\]

for \( i = 1, \ldots, n - 1 \).

It is noted that \( h_i \) is continuous on \( U_i = [-\delta_N, \delta_N] \) and differentiable on \((\delta_N, \delta_N)\) for \( i = 1, \ldots, n - 1 \) and \( f^* \) is continuous and differentiable on \( S^* \). Composition of two continuous functions is continuous and the composition of two differentiable functions is differentiable. Hence, \( g_i \) is continuous on \( U_i = [-\delta_N, \delta_N] \) and differentiable on \((\delta_N, \delta_N)\).

Take any \( i \in \{1, \ldots, n - 1\} \). Note that \( g_i(\delta_N) = f^*(\mathbf{u}_N^{(i+)}), g_i(-\delta_N) = f^*(\mathbf{u}_N^{(i-)}), g_i(0) = f^*(\mathbf{u}^*) \). So, \( g_i(0) \leq g_i(-\delta_N) \) and \( g_i(0) \leq g_i(\delta_N) \). Without loss of generality, assume \( f^*(\mathbf{u}_N^{(i+)}') \leq f^*(\mathbf{u}_N^{(i-)}') \) which implies \( g_i(0) \leq g_i(-\delta_N) \leq g_i(\delta_N) \).

Since we have \( g_i(0) \leq g_i(-\delta_N) \leq g_i(\delta_N) \), from continuity of \( g_i \) we can say that there exists \( w \in [0, \delta_N] \) such that \( g_i(w) = g_i(-\delta_N) \geq g_i(0) \). Now \( g_i \) is continuous on \([-\delta_N, \delta_N] \) and differentiable on \((\delta_N, \delta_N)\) implies \( g_i \) is continuous on \([-\delta_N, w] \) and differentiable on \((-\delta_N, w)\). Using Mean value theorem we can say that there exists a point \( v \in [-\delta_N, w] \) such that \( g_i'(v) = 0 \). We claim that \( g_i'(v) = 0 \) holds for \( v = 0 \).
Suppose \( g'_0 \neq 0 \). Assume \( g'_0(v^*) = 0 \) for some \( v^* \neq 0 \) and \( v^* \in (-\delta_N, w) \). Without loss of generality, we assume \( v^* > 0 \). Since \( h_i \) and \( f \) are convex, \( g_i \) is also convex. Now \( g'_0(v^*) = 0 \) implies \( v^* \) is a local minima. On the other hand, since \( g'_0(0) \neq 0 \), implies 0 is not a critical point or local minima. Hence, \( g_i(0) > g_i(v^*) \). Take \( N_1 \in \mathbb{Z} \) such that \( 0 < \delta N_1 < v^* \). Hence there exists a \( \lambda \in (0, 1) \) such that \( \delta N_1 = \lambda.0 + (1 - \lambda).v^* \). Now,

\[
g_i(\delta N_1) = g_i(\lambda.0 + (1 - \lambda).v^*) \leq \lambda g_i(0) + (1 - \lambda)g_i(v^*) = g_i(0) + (1 - \lambda)(g_i(v^*) - g_i(0)) = g_i(0) - (1 - \lambda)(g_i(0) - g_i(v^*)) < g_i(0).
\]

But, we know for all \( k \in \mathbb{Z} \), \( g_i(0) \leq g_i(\delta_k) \) which implies \( g_i(0) \leq g_i(\delta N_1) \). It is a contradiction. Hence we have \( g'_0(0) = 0 \). Now

\[
g'_0(0) = \left[ \frac{\partial}{\partial \epsilon} g_i(\epsilon) \right]_{\epsilon=0} = \left[ \frac{\partial}{\partial \epsilon} f^*(h_i(\epsilon)) \right]_{\epsilon=0} = \left[ \frac{\partial}{\partial h_i(\epsilon)} f^*(h_i(\epsilon)) \right]_{\epsilon=0} \left[ \frac{\partial}{\partial \epsilon} h_i(\epsilon) \right]_{\epsilon=0}.
\]

Now \( h_i(0) = u^* \). Hence

\[
\left[ \frac{\partial}{\partial h_i(\epsilon)} f^*(h_i(\epsilon)) \right]_{\epsilon=0} = \nabla f^*(u^*) = \left[ \frac{\partial}{\partial x_1} f^*(u^*), \ldots, \frac{\partial}{\partial x_{n-1}} f^*(u^*) \right] = \left[ \nabla_1, \ldots, \nabla_{n-1} \right]
\]

where \( \nabla_i = \frac{\partial}{\partial x_i} f^*(u^*) \) for \( i = 1, \ldots, n-1 \). and

\[
\frac{\partial}{\partial \epsilon} h_i(\epsilon) = [a_{i1}, \ldots, a_{i(n-1)}]^T
\]

where \( a_{ii} = 1 \) and \( a_{ij} = -\frac{1}{n-1} \) for \( j \in \{1, \ldots, n-1\} \setminus \{i\} \) Hence

\[
\left[ \frac{\partial}{\partial \epsilon} g_i(\epsilon) \right]_{\epsilon=0} = \left[ \nabla_1, \ldots, \nabla_{n-1} \right] [a_{i1}, \ldots, a_{i(n-1)}]^T = \left[ a_{i1}, \ldots, a_{i(n-1)} \right] \begin{bmatrix} \nabla_1 \\ \vdots \\ \nabla_{n-1} \end{bmatrix} = 0.
\]
Since this equation holds for all $i = 1, \ldots, n - 1$, we have $Ax = 0$ where

$$A_{n \times n} = \begin{bmatrix}
    1 & -\frac{1}{n-1} & \cdots & -\frac{1}{n-1} \\
    -\frac{1}{n-1} & 1 & \cdots & -\frac{1}{n-1} \\
    \vdots & \vdots & \ddots & \vdots \\
    -\frac{1}{n-1} & -\frac{1}{n-1} & \cdots & 1
\end{bmatrix}, x_{n \times 1} = \begin{bmatrix}
    \nabla_1 \\
    \vdots \\
    \nabla_{n-1}
\end{bmatrix}.$$

Since $A$ is full rank for $n \in \mathbb{N}\setminus\{1\}$, $Ax = 0$ implies $x = 0$. Hence $\frac{\partial}{\partial x_i} f^*(u^*) = 0$ for all $i = 1, \ldots, n - 1$. Hence $u^*$ is a critical point. Since $f^*$ is convex, a local minima occurs at $u^*$. But for a convex function, global minimum occurs at any local minimum. Hence global minimum of $f^*$ occurs at $u^*$, which clearly implies global minimum of $f$ occurs at $u$.

Suppose the solution given by GCDVSS is a point $u \in S$ such that all it’s coordinates are greater than zero. Our algorithm stops and yields the final solution when two consecutive runs give the same solution. It implies in the last run, for all movements of step sizes $\delta_k = \frac{\text{maximal}}{\rho^k}$ (until $\delta_k$ gets smaller than the step size threshold) the objective function value is checked at $u^{(i+)}_k, u^{(i-)}_k$ and $f(u) \leq f(u^{(i+)}_k)$ and $f(u) \leq f(u^{(i-)}_k)$ hold for all $i = 1, \ldots, n$. So taking step size threshold small enough, this algorithm reaches the global minimum under assumed regularity conditions of the objective function. Note that, ideally the value of $\lambda$ should be taken to be zero. But, in practical, it is noted that setting a small non-zero value of $\lambda$ (specially in high-dimensional problems with possibility of sparsity) increases the efficiency and accuracy of the solution provided by this algorithm.

5 Generalization to some other cases

In this section the proposed algorithm has been extended for two general cases, namely simplex inequality and single linearly constrained parameter space.

5.1 Simplex Inequality

Consider the case where the optimization problem is given by

$$\begin{align*}
\text{minimize} & : f(p_1, \ldots, p_m) \\
\text{subject to} & : p_i \geq 0, 1 \leq i \leq m, \sum_{i=1}^m p_i \leq 1.
\end{align*}$$

\hspace{1cm} (4)

Under this scenario, a slack variable $p_{m+1}$ is introduced such that $p_{m+1} \geq 0$ and $\sum_{i=1}^{m+1} p_i = 1$. Define $f_1(p_1, \ldots, p_{m+1}) = f(p_1, \ldots, p_m)$. So, the modified
optimization problem which is equivalent to Equation (4) is given by

\[
\begin{align*}
\text{minimize} & : f_1(p_1, \cdots, p_{m+1}) \\
\text{subject to} & : p_i \geq 0, \ 1 \leq i \leq m+1, \ \sum_{i=1}^{m+1} p_i = 1,
\end{align*}
\]

which can be easily solved using the proposed algorithm.

5.2 Linear Constraint with Positive Coefficients

Now, consider the case where the optimization problem is as following

\[
\begin{align*}
\text{minimize} & : f(x_1, \cdots, x_m) \\
\text{subject to} & : x_i \geq 0, \ 1 \leq i \leq m, \ \sum_{i=1}^{m} a_i x_i = K,
\end{align*}
\]

where \(\{a_i\}_{i=1}^{m}, K\) are given positive constants. To solve this problem, consider the change of variable given by \(y_i = \frac{a_i x_i}{K}\) for \(i = 1, \ldots, m\). \(y_i\) is non-negative since \(K > 0, x_i \geq 0\) and \(a_i > 0\) for \(i = 1, \ldots, m\). Now, \(\sum_{i=1}^{m} a_i x_i = K\) is equivalent to \(\sum_{i=1}^{m} y_i = 1\). Consider the mapping \(g : \mathbb{R}^m \mapsto \mathbb{R}^m\)

\[
g(y_1, \ldots, y_m) = \left(\frac{Ky_1}{a_1}, \ldots, \frac{Ky_m}{a_m}\right).
\]

Define \(h : \mathbb{R}^m \mapsto \mathbb{R}\) such that \(h = f \circ g\). So,

\[
h(y_1, \ldots, y_m) = f(g(y_1, \ldots, y_m)) = f\left(\frac{Ky_1}{a_1}, \ldots, \frac{Ky_m}{a_m}\right) = f(x_1, \ldots, x_m).
\]

Hence, the optimization problem in Equation (6) is equivalent to

\[
\begin{align*}
\text{minimize} & : h(y_1, \cdots, y_m) \\
\text{subject to} & : y_i \geq 0, \ 1 \leq i \leq m, \ \sum_{i=1}^{m} y_i = 1,
\end{align*}
\]

which can be solved using the proposed algorithm.
6 Application to non-convex global optimization on Simplex

In this section, we compare the performance of the proposed method (GCD-VSS) to three standard constrained optimization methods: the ‘interior-point’ (IP) algorithm, ‘sequential quadratic programming’ (SQP) and ‘genetic algorithm’ (GA) for optimization of non-convex problems on simplex parameter space. All of the above-mentioned well-known algorithms are available in Matlab R2014a (The Mathworks) via the Optimization Toolbox functions \texttt{fmincon} (for IP and SQP algorithm) and \texttt{ga} (for GA). IP and SQP search for local minimum and they are less time consuming in general. On the other hand GA tries to find global minimum, being more time consuming. In the following studies, we considered the convergence to the true solution to be successful if the absolute distance of the optimum objective function value returned by the algorithms with the true optimum value of the objective function is less than $10^{-2}$. For GCDVSS algorithm, the values of all the tuning parameters have been taken to be same as mentioned in Section 2. For IP and SQP algorithms, the upper bound for maximum number of iterations and function evaluations is set to be infinity each. For GA, we use the default options of ‘ga’ function in Matlab R2014a. GCDVSS algorithm is implemented in Matlab R2014a. We perform the simulations in a machine with 64-Bit Windows 8.1, Intel i7 3.60GHz processors and 32GB RAM.

6.1 Maximum of two Gaussian densities

Consider the problem

maximize : $\max \{ 8 \ast \phi(\mathbf{p}; \mu_1, \Sigma_1), 5 \ast \phi(\mathbf{p}; \mu_2, \Sigma_2) \}$
subject to : $p_1, p_2 \geq 0, \quad p_1 + p_2 = 1$ \hspace{1cm} (8)

where $\mathbf{p} = (p_1, p_2)$ is our parameter of interest, $\phi(\mathbf{x}; \mu, \Sigma)$ denotes the normal density at $\mathbf{x}$ with mean $\mu$ and covariance matrix $\Sigma$. Here, $\mu_1 = \begin{bmatrix} 0.25 \\ 0.75 \end{bmatrix}$, $\mu_2 = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix}$ and $\Sigma_1 = \Sigma_2 = \begin{bmatrix} 0.1 & 0 \\ 0 & 0.1 \end{bmatrix}$. In Figure 1(b) we plot the function on the restricted parameter space. Note that is has two local maximas at $(p_1, p_2) = (0.8, 0.2)$ and $(0.25, 0.75)$. Out of these two points, the global maxima occurs at $(0.25, 0.75)$. For comparative study, we take starting point $(p_1, p_2) = (0.8, 0.2)$ (which is a local maxima, not the global maxima) for GCDVSS, SQP, IP and GA. Starting from this point, it is to be noted that the global maxima $(0.25, 0.75)$ is reached using GCDVSS and GA algorithms only and the average (over 100 repetitions) time required for convergence are 0.07 and 1.52 seconds respectively. While using IP and SQP algorithms, the starting point being the local maxima, is returned as the final solution and hence the global maxima is not achieved. We also perform a comparison study between these four methods, starting from 100 randomly generated points satisfying the simplex constraint. In Table 1 it is noted that out of 100 times, every time GCDVSS and GA
reach the global maxima and GCDVSS is (on average) 21 times faster than GA. SQP and IP reaches the global maxima 67 and 71 times respectively out of 100 times.

6.2 Modified Easom function on simplex

Consider the following problem

\[
\text{maximize : } \cos(6\pi p_1) \cos(6\pi p_2) \cos(6\pi p_3) \exp(-\sum_{i=1}^{3}(3\pi p_i - \pi)^2)
\]
\[\text{subject to : } p_1, p_2, p_3 \geq 0, \ \ p_1 + p_2 + p_3 = 1 \quad (9)
\]

This function has multiple local maxima (see Figure 2) with the global maxima at \(p = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\), the functional value at this point being 1. Starting from randomly generated 100 points within the domain of simplex, the result of the comparative study of all above-mentioned algorithms have been shown in Table 1. It is noted that GCDVSS is around 85 times faster than GA.

6.3 Non-linear non-convex optimization on 2-simplex

Here we consider a problem of non-linear non-convex function optimization on the a linearly constrained space on \(\mathbb{R}^2\).

\[
\text{maximize : } \sin(\frac{7\pi x}{4}) + \sin(\frac{7\pi y}{4}) - 2(x - y)^2
\]
\[\text{subject to : } 3x + 2y \leq 6, \ \ x, y \geq 0 \quad (10)
\]

In Figure 3(a), we plot a heat-map of the values of this function over the parameter space. It can be easily noted that there exist 4 local maxima of
which the global maximum occurs at \((x, y) = \left(\frac{2}{3}, \frac{2}{3}\right) = (0.2857, 0.2857)\), the objective function value being 2 at this point. Note that it can be considered as an optimization problem on simplex. Because, any point in the feasible region is in the convex hull generated by \((0, 0)\), \((2, 0)\) and \((0, 3)\) on \(\mathbb{R}^2\). In Table 1, we note that GCDVSS outperforms the other algorithms based on the comparative study of the number of successful convergences for all methods starting from 100 randomly generated starting points.
Table 1 Comparison of required time and number of successful convergence for solving the problems in Example (6.1), (6.2) and (6.3) using GCDVSS, SQP, IP and GA starting from 100 randomly generated points.

| Algorithms | Example [6.1] | Example [6.2] | Example [6.3] |
|------------|---------------|---------------|---------------|
|            | Success (%)   | Avg. Time (sec) | Success (%)   | Avg. Time (sec) | Success (%)   | Avg. Time (sec) |
| GCDVSS     | 100           | 0.071         | 100           | 0.016         | 100           | 0.019         |
| SQP        | 67            | 0.014         | 31            | 0.014         | 44            | 0.025         |
| IP         | 71            | 0.023         | 47            | 0.030         | 47            | 0.014         |
| GA         | 100           | 1.494         | 100           | 1.354         | 100           | 1.270         |

Table 2 Comparison of required time and number of successful convergence for solving the problem in Example (6.4) using GCDVSS, SQP, IP and GA for \( n = 5, 10, 25, 50, 100 \) starting from 100 randomly generated points in each case.

| Algorithms | \( n=5 \) | \( n=10 \) | \( n=25 \) | \( n=50 \) | \( n=100 \) |
|------------|-----------|-----------|-----------|-----------|-----------|
|            | No. of success | Avg. time | No. of success | Avg. time | No. of success | Avg. time | No. of success | Avg. time | No. of success | Avg. time |
| GCDVSS     | 100        | 0.000     | 100        | 0.000     | 100        | 0.000     | 100        | 0.000     | 100        | 0.000     |
| SQP        | 31         | 0.008     | 22         | 0.010     | 16         | 0.017     | 15         | 0.028     | 7          | 0.061     |
| IP         | 30         | 0.022     | 22         | 0.026     | 15         | 0.052     | 22         | 0.094     | 26         | 0.181     |
| GA         | 4          | 2.950     | 0          | 25.762    | 0          | 3.191     | 0          | 50.385    | 0          | 51.232     |

6.4 Optimization of function with multiple local extremums on boundary points for various dimensions

Consider the problem

\[
\text{maximize : } \sum_{i=1}^{n} i p_i^4 \\
\text{subject to : } p_i \geq 0, \ i = 1, \cdots, n \sum_{i=1}^{n} p_i = 1 (11)
\]

where \( n \) is any positive integer. This function has local maximas at the boundary points of the simplex. But the global maxima occurs at \( \mathbf{p} = (p_1, \cdots, p_n) \) for \( p_1 = \cdots = p_{n-1} = 0 \) and \( p_n = 1 \). The objective function value at this point is equal to \( n \). With increasing value of \( n \), it gets harder to estimate the global maxima. In Figure 3(b) we plot the heat map of \( f(\mathbf{p}) \) for \( n = 3 \). It can be seen that this function has three local maxima at \( P_1 = (1, 0, 0), P_2 = (0, 1, 0) \) and \( P_3 = (0, 0, 1) \) where \( P_3 = (0, 0, 1) \) is the global maxima. For each \( n = 5, 10, 25, 50, 100 \), we perform a comparative study of performances of all the above-mentioned algorithms starting from randomly generated 100 points within corresponding domain. In Table (2), we note that unlike GA, GCDVSS works well for high-dimensional cases also. In higher dimensions, GCDVSS outperforms GA significantly. It is also noted that the required time of computation for GCDVSS algorithm increases almost linearly with dimension of the problem.
6.5 Transformed Ackley’s Function on Simplex

Consider an unconstrained function $f$ needs to be minimized on a $d$-dimensional hypercube $D^d$ where $D = [l, u]$ for some constants $l, u$ in $\mathbb{R}$. Consider the bijective map $g : D \rightarrow [0, \frac{1}{d}]$ such that $g(x_i) = y_i = \frac{x_i - l}{u - l}$ for $i = 1, \ldots, d$. Replacing the original parameters of the problem with the transformed parameters we get

$$f(x_1, \ldots, x_d) = f(g^{-1}(y_1), \ldots, g^{-1}(y_d)).$$

Now, define $h : [0, \frac{1}{d}]^d \rightarrow \mathbb{R}$ such that

$$h(y_1, \ldots, y_d) = f(g^{-1}(y_1), \ldots, g^{-1}(y_d)).$$

Consider the set $S = \{(z_1, \ldots, z_d) \mid z_i \geq 0, \sum_{i=1}^d z_i \leq 1\}$. Clearly $[0, \frac{1}{d}]^d \subset S$. Define $h' : S \rightarrow \mathbb{R}$ which is equal to function $h$ considered on the extended domain $S$. We have $y_i \in [0, \frac{1}{d}]$ for $i = 1, \ldots, d$ and $0 \leq \sum_{i=1}^d y_i \leq 1$. Define $y_{d+1} = 1 - \sum_{i=1}^d y_i$. Clearly, $0 \leq y_{d+1} \leq 1$ and $\sum_{i=1}^{d+1} y_i = 1$. Hence we can conclude that $y = (y_1, \ldots, y_d)$ and

$$\Delta^d = \{(y_1, \ldots, y_{d+1}) \in \mathbb{R}^{d+1} \mid y_i \geq 0, i = 1, \ldots, d+1, \sum_{i=1}^{d+1} y_i = 1\}.$$

Now define $\bar{h} : \Delta^d \rightarrow \mathbb{R}$ such that $\bar{h}(\bar{y}) = \bar{h}(y_1, \ldots, y_{d+1}) = h'(y_1, \ldots, y_d)$ for $\bar{y} \in \Delta^d$. It can be seen that $\bar{y} \in \Delta^d$ implies $(y_1, \ldots, y_d) \in S$. Suppose the global minimum of the function $f$ occurs at $(m_1, \ldots, m_d)$ in $D^d$. Hence, the function $\bar{h}$ will have the global minimum at $\bar{y} = (g^{-1}(m_1), \ldots, g^{-1}(m_d), 1 - \sum_{i=1}^d g^{-1}(m_i))$ in $\Delta^d$.

$d$-dimensional Ackley’s function is given by

$$f(x_1, \ldots, x_d) = -20 \exp(-0.2 \sqrt{\frac{1}{d} \sum_{i=1}^d x_i^2}) - \exp(0.5 \sum_{i=1}^d \cos(2\pi x_i)) + e + 20$$

The domain of $x = (x_1, \ldots, x_d)$ is generally taken to be $[-5, 5]^d$. The global minimum of $f$ is 0 (even if considered on $\mathbb{R}^d$) which occurs at $x^* = (x_1^*, \ldots, x_d^*) = (0, \ldots, 0)$. After doing the above mentioned transformations taking $l = -5$ and $u = 5$, we get the transformed Ackley’s function on a $d$-dimensional unit-simplex $\Delta^d$ given by

$$\bar{h}(\bar{y}) = -20 \exp(-0.2 \sqrt{\frac{1}{d} \sum_{i=1}^d (g^{-1}(y_i))^2} - \exp(0.5 \sum_{i=1}^d \cos(2\pi g^{-1}(y_i))) + e + 20$$

The global minimum of the transformed Ackley’s function on simplex occurs at $\bar{y}^*_1 \times \Delta^d = (\frac{1}{2\pi}, \ldots, \frac{1}{2\pi}, 1)$ which is found using inverse transformation on $x^*$ as
mentioned above. For comparative study we considered GCDVSS algorithm for three set of parameter with default parameter values (as mentioned in Section 2) and two more set of parameter values which are GCDVSS (pl1) and GCDVSS (pl2) (pl stands for precision level). In GCDVSS (pl1), we take $\lambda = \phi = 10^{-5}$ and for GCDVSS (pl2), we take $\lambda = \phi = 10^{-7}$ keeping the values of the other parameters same as default. For each algorithm, transformed Ackley’s function has been optimized for $d = 5, 10, 25, 50$ and $100$. In each case, the objective function has been minimized starting from $100$ randomly chosen points. In Table 3, the average computation time and the minimum value achieved for each algorithm have been given. It is noted that for this function, GCDVSS algorithm outperforms all other algorithms significantly. It is also observed that taking smaller values of $\lambda$ and $\phi$ improves the accuracy of the solution at the cost of higher computation time. For $d = 5$, GCDVSS (pl1) yields better solution than GA with a $235$ folds improvement in average computation time.

6.6 Transformed Griewank’s Function on Simplex

d-dimensional Griewank’s function is given by

$$f(x_1, \ldots, x_d) = \frac{1}{4000} \sum_{i=1}^{d} x_i^2 - \prod_{i=1}^{d} \cos \left( \frac{x_i}{\sqrt{i}} \right) + 1$$

The domain of $x = (x_1, \ldots, x_d)$ is generally taken to be $[-500, 500]^d$. The global minimum of $f$ is $0$ (even if considered on $\mathbb{R}^d$) which occurs at $x^* = (x^*_1, \ldots, x^*_d) = (0, \ldots, 0)$. Similar to the previous problem, after performing the above mentioned transformations taking $l = -500$ and $u = 500$, we get the transformed Griewank’s function on a $d$-dimensional unit-simplex $\Delta^d$ given by

$$\bar{h}(\bar{y}) = \bar{h}(y_1, \ldots, y_{d+1}) = \frac{1}{4000} \sum_{i=1}^{d} (g^{-1}(y_i))^2 - \prod_{i=1}^{d} \cos \left( \frac{g^{-1}(y_i)}{\sqrt{i}} \right) + 1$$

Like the previous function, in this case also the transformed global minimum occurs at $\bar{y}_1^{* \times (d+1)} = (\frac{1}{\sqrt{d}}, \ldots, \frac{1}{\sqrt{d}}, \frac{1}{\sqrt{d}})$. Simulation study has been performed for this function under the similar setup of Example (6.5). In this case, although SQP and IP performs better than GCDVSS (default, pl1 & pl2) and GA for smaller dimensional cases but GCDVSS (pl1 & pl2) performs same or better than other algorithms in high-dimensional problems. In this case also, the solution improves taking the values of $\lambda$ and $\phi$ smaller. Note that for $d = 5$, there has been more than $338$ folds improvement in average computation time on using GCDVSS(pl1) over GA along with more accuracy.
6.7 Transformed Rastrigin’s Function on Simplex

d-dimensional Rastrigin’s function is given by

\[ f(x_1, \ldots, x_d) = 10d + \sum_{i=1}^{d} [x_i^2 - 10 \cos(2\pi x_i)] \]

The domain of \( x = (x_1, \ldots, x_d) \) is generally taken to be \([-5, 5]^d\). After transformation in the above-mentioned way, the transformed Rastrigin’s function on \( \Delta^d \) is given by

\[ \bar{h}(y) = \bar{h}(y_1, \ldots, y_{d+1}) = 10d + \sum_{i=1}^{d} [(g^{-1}(y_i))^2 - 10 \cos(2\pi g^{-1}(y_i))] \]

The global minimum of \( \bar{h} \) occurs at \( y_1^{\ast} = (\frac{1}{2}, \ldots, \frac{1}{2}) \) which follows from the fact that the global minimum of the original form of Rastrigin’s function occurs at \( x^* = (x_1^*, \ldots, x_d^*) = (0, \ldots, 0) \). Comparative study of performances of the algorithms has been carried out for this function under the same setup of (6.5). In Table 3 it is noted that GCDVSS outperforms other algorithms significantly. It is noticeable that for \( d = 5 \), GCDVSS (pl2) gives more accurate solution than GA with a 253 folds improvement in average computation time.

7 Discussion

This paper has presented a novel efficient derivative-free algorithm for global optimization of any objective function whose parameters are on simplex. This algorithm being derivative-free, is efficient when the closed form of derivative does not exist or it is expensive to evaluate. Unlike other global optimization techniques (e.g., genetic algorithm), the number of required function evaluations for this algorithm increases only in the order of the number of parameters which makes it work faster for high dimensional problems. The way this algorithm evaluates the objective function value at different sites of the sample space, incorporation of parallelization can be done easily making the algorithm even faster for expensive high dimensional objective functions. The requirement of parallelization only increases linearly with the number of parameters.

Another unique feature of this algorithm is, unlike other global optimizers (e.g., genetic algorithm) this algorithm works fast enough for simpler and convex optimization problems. Also it guarantees the global solution when the function is convex, continuous and differentiable on the simplex domain.

The accuracy of the solution can be controlled changing the values of the tuning parameters. In Example (6.5), (6.6) and (6.7) it is noted that smaller
Table 3 Comparison of minimum value achieved and average computation time (in seconds) for solving transformed \(d\)-dimensional Ackley's function, Griewank's function and Rastrigin's function on simplex for \(d = 5, 10, 25, 50\) and 100 using GCDVSS (default, lp1 & lp2), SQP, IP and GA for \(d = 5, 10, 25, 50, 100\) starting from 100 randomly generated points in each case.

| Functions                  | Algorithms | \(d = 5\)                  | \(d = 10\)                  | \(d = 25\)                  | \(d = 50\)                  | \(d = 100\)                  |
|----------------------------|------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
|                            |            | Min. value | Avg. time | Min. value | Avg. time | Min. value | Avg. time | Min. value | Avg. time | Min. value | Avg. time |
| Ackley's Function (transformed) | GCDVSS     | 3.24e - 02 | 0.099     | 1.16e - 01 | 0.199     | 3.74e - 01 | 0.546     | 9.24e - 01 | 1.189     | 1.34e - 00 | 3.685     |
|                            | GCDVSS (pl1) | 2.88e - 04 | 0.163     | 4.91e - 04 | 0.314     | 2.59e - 03 | 0.876     | 5.15e - 03 | 2.234     | 1.08e - 02 | 6.277     |
|                            | GCDVSS (pl2) | 1.31e - 06 | 0.186     | 6.45e - 06 | 0.394     | 2.47e - 05 | 1.194     | 4.97e - 05 | 3.063     | 1.04e - 04 | 9.307     |
|                            | SQP        | 1.65e - 00 | 0.032     | 2.01e - 00 | 0.090     | 4.71e - 00 | 0.192     | 1.73e - 00 | 0.541     | 1.27e - 00 | 2.861     |
|                            | IP         | 2.32e - 00 | 0.078     | 2.32e - 00 | 0.139     | 8.58e - 00 | 0.361     | 1.32e + 01 | 0.865     | 1.49e + 01 | 2.863     |
|                            | GA         | 8.46e - 04 | 38.395    | 3.60e - 00 | 40.653    | 1.12e + 01 | 40.097    | 1.44e + 01 | 39.761    | 1.60e + 01 | 46.626    |

| Griewank's Function (transformed) | GCDVSS     | 8.39e - 02 | 0.069     | 6.44e - 01 | 0.103     | 1.25e - 00 | 0.322     | 2.81e - 00 | 0.795     | 1.30e + 01 | 2.152     |
|                                 | GCDVSS (pl1) | 7.65e - 03 | 0.111     | 8.87e - 03 | 0.213     | 6.24e - 03 | 0.599     | 2.60e - 02 | 1.518     | 9.12e - 02 | 5.609     |
|                                 | GCDVSS (pl2) | 7.40e - 03 | 0.136     | 7.40e - 03 | 0.248     | 4.87e - 07 | 0.808     | 2.64e - 06 | 2.186     | 1.24e - 05 | 6.345     |
|                                 | SQP        | 3.73e - 01 | 0.041     | 8.84e - 09 | 0.084     | 6.70e - 08 | 0.267     | 1.24e - 05 | 0.784     | 3.15e - 04 | 3.138     |
|                                 | IP         | 2.04e - 01 | 0.129     | 2.33e - 09 | 0.174     | 2.47e - 08 | 0.294     | 1.86e - 07 | 0.586     | 1.23e - 06 | 1.802     |
|                                 | GA         | 1.94e - 02 | 37.578    | 1.23e + 01 | 37.765    | 7.52e + 01 | 38.598    | 3.52e + 03 | 40.148    | 1.06e + 04 | 46.527    |

| Rastrigin's Function (transformed) | GCDVSS     | 1.25e - 00 | 0.068     | 2.68e - 00 | 0.125     | 9.21e - 00 | 0.300     | 1.60e + 01 | 0.859     | 4.77e + 01 | 2.349     |
|                                   | GCDVSS (pl1) | 3.07e - 05 | 0.118     | 3.98e - 00 | 0.211     | 2.61e - 03 | 0.640     | 9.97e - 00 | 1.453     | 6.15e - 00 | 4.213     |
|                                   | GCDVSS (pl2) | 1.51e - 09 | 0.163     | 3.98e - 00 | 0.333     | 2.55e - 07 | 0.929     | 9.95e - 01 | 2.084     | 5.97e - 00 | 6.014     |
|                                   | SQP        | 2.98e - 00 | 0.030     | 2.19e + 01 | 0.062     | 1.79e + 02 | 0.230     | 4.05e + 02 | 0.718     | 6.85e + 02 | 3.578     |
|                                   | IP         | 9.95e - 00 | 0.076     | 6.17e + 01 | 0.138     | 2.01e + 02 | 0.947     | 4.25e + 02 | 15.196    | 8.04e + 02 | 3.342     |
|                                   | GA         | 6.8e - 06  | 41.271    | 3.24e + 01 | 40.772    | 4.68e + 02 | 40.730    | 1.88e + 03 | 42.553    | 5.32e + 03 | 45.797    |
values of step size threshold ($\phi$) and sparsity threshold ($\lambda$) improves solution accuracy in the cost of higher computation time. In case of beforehand knowledge of sparsity (specially in high-dimensional simplex), increasing sparsity threshold results in better solution with relatively lower computation time. Under the default values of the tuning parameters (described in Section 2), it is shown that this algorithm outperforms SQP, IP and GA for optimizing various non-convex functions on simplex. For higher dimensional problems, setting lower values of $\lambda$ and $\phi$ is recommended for improving the performance of the proposed algorithm.

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