

A Two-phase Framework with a Bézier Simplex-based Interpolation Method for Computationally Expensive Multi-objective Optimization

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ABSTRACT

This paper proposes a two-phase framework with a Bézier simplex-based interpolation method (TPB) for computationally expensive multi-objective optimization. The first phase in TPB aims to approximate a few Pareto optimal solutions by optimizing a sequence of single-objective scalar problems. The first phase in TPB can fully exploit a state-of-the-art single-objective derivative-free optimizer. The second phase in TPB utilizes a Bézier simplex model to interpolate the solutions obtained in the first phase. The second phase in TPB fully exploits the fact that a Bézier simplex model can approximate the Pareto optimal solution set by exploiting its simplex structure when a given problem is simplicial. We investigate the performance of TPB on the 55 bi-objective BBOB problems. The results show that TPB performs significantly better than HMO-CMA-ES and some state-of-the-art meta-model-based optimizers.

CCS CONCEPTS

• **Mathematics of computing** → **Evolutionary algorithms.**

KEYWORDS

Multi-objective numerical optimization, Bézier simplices

ACM Reference Format:

Ryoji Tanabe, Youhei Akimoto, Ken Kobayashi, Hiroshi Umeki, Shinichi Shirakawa, and Naoki Hamada. 2022. A Two-phase Framework with a Bézier Simplex-based Interpolation Method for Computationally Expensive Multi-objective Optimization. In *Genetic and Evolutionary Computation Conference (GECCO '22)*, July 9–13, 2022, Boston, MA, USA. ACM, New York, NY, USA, 10 pages. <https://doi.org/10.1145/3512290.3528778>

1 INTRODUCTION

General context. This paper considers computationally expensive multi-objective black-box numerical optimization. Some real-world

optimization problems require computationally expensive simulation to evaluate the solution (e.g., [17, 64]). In this case, only a limited budget of function evaluations is available for multi-objective optimization. Instead of general evolutionary multi-objective optimization (EMO) algorithms (e.g., NSGA-II [18] and MOEA/D [65]), meta-model-based approaches [15, 58] have been generally used for computationally expensive multi-objective optimization.

Some mathematical derivative-free optimizers (e.g., NEWUOA [52], BOBYQA [53], and SLSQP [44]) have shown their effectiveness for computationally expensive *single-objective* black-box numerical optimization. For example, Hansen et al. [31] investigated the performance of 31 optimizers on the noiseless BBOB function set [33]. Their results showed that NEWUOA achieves the best performance in the 31 optimizers for a small number of function evaluations. The results in [51, 55] also reported the excellent convergence performance of NEWUOA. The results in [29] demonstrated that SLSQP can quickly find the optimal solution on some unimodal functions. In [2], Bajer et al. showed that BOBYQA outperforms some meta-model-based optimizers including SMAC [39] and Imm-CMA [7].

Motivation. Let $g_{\mathbf{w}} : \mathbb{R}^M \rightarrow \mathbb{R}$ be a scalarizing function that maps an M -dimensional objective vector to a scalar value. Let also $\mathbf{W} = \{\mathbf{w}_k\}_{k=1}^K$ be a set of K uniformly distributed weight vectors. Under certain conditions, the optimal solution of a single-objective scalar optimization problem can be a weakly Pareto optimal solution (see Chapter 3.5 in [48]). Therefore, K weakly Pareto optimal solutions can potentially be obtained by solving a sequence of K single-objective scalar optimization problems $\{g_{\mathbf{w}_k}\}_{k=1}^K$. Any single-objective optimizer can be applied to the K scalar optimization problems in principle. When the number of function evaluations is limited, a mathematical derivative-free optimizer is likely to be suitable for this purpose based on the above review.

Actually, the first warm start phase in HMO-CMA-ES [45] adopts this idea. HMO-CMA-ES was designed to achieve good anytime performance for bi-objective optimization in terms of the hypervolume indicator [67]. HMO-CMA-ES is a hybrid multi-objective optimizer that consists of four phases. The first out of the four phases in HMO-CMA-ES applies BOBYQA to a sequence of K scalar optimization problems $\{g_{\mathbf{w}_k}\}_{k=1}^K$ for only the first $10 \times N$ function

evaluations, where N is the number of variables. Let X be the set of all solutions found so far by BOBYQA. At the end of the first phase, HMO-CMA-ES selects five solutions from X by applying environmental selection in SMS-EMOA [3]. Then, the second phase in HMO-CMA-ES performs a steady-state MO-CMA-ES [40] with the initial population of the five solutions. Brockhoff et al. [9] showed that HMO-CMA-ES performs significantly better than some multi-objective optimizers for the first $10 \times N$ function evaluations, including NSGA-II [18], COMO-CMA-ES [61], and DMS [16]. Thus, their results indicate the effectiveness of mathematical derivative-free approaches to solving a scalar problem for computationally expensive multi-objective optimization.

One drawback of the above-discussed scalar optimization approach is that it can achieve only K solutions that are sparsely distributed in the objective space, even in the best case. Since only a limited number of function evaluations are available for computationally expensive optimization, K needs to be as small as possible. Due to the small value of K , the above-discussed scalar optimization approach cannot obtain a set of non-dominated solutions that cover the entire Pareto front in the objective space.

However, we believe that the issue of the above-discussed scalar optimization approach can be addressed by using a solution interpolation method. Let $X = \{x_k\}_{k=1}^K$ be a set of K solutions obtained by optimizing a sequence of K single-objective scalar optimization problems $\{g_{w_k}\}_{k=1}^K$. Densely distributed solutions in the objective space can potentially be obtained by interpolating the K sparsely distributed solutions in X . Some solution interpolation methods have been proposed in the literature (see Section 3). Unfortunately, existing methods were not designed for interpolating only a few (say $K \in \mathcal{O}(M)$) solutions. In addition, we are particularly interested in optimization with a small budget of function evaluations.

The Bézier simplex is an extended version of the Bézier curve [23] to higher dimensions. For a certain class of problems, the Bézier simplex has a capability to interpolate K solutions, approximating the entire set of Pareto optimal solutions. More precisely, Hamada et al. [27] showed that the set of Pareto optimal solutions is homeomorphic to an $(M-1)$ -dimensional simplex under certain conditions. In such a case, Kobayashi et al. [43] proved that a Bézier simplex model can approximate the Pareto optimal solution set. They also proposed an algorithm for fitting a Bézier simplex by extending the Bézier curve fitting [6]. Their results in [43] demonstrated that it achieved an accurate approximation with a small number of solutions. Thus, we expect that the Bézier simplex model can effectively interpolate the K sparsely distributed solutions.

Contribution. Motivated by the above discussion, this paper proposes a two-phase framework with a Bézier simplex-based interpolation method (TPB) for computationally expensive multi-objective black-box optimization. The first phase performs a mathematical derivative-free optimizer on a sequence of K single-objective scalar optimization problems $\{g_{w_k}\}_{k=1}^K$. The second phase fits a Bézier simplex model to the K solutions obtained in the first phase. Then, TPB samples interpolated solutions from the Bézier simplex model. We investigate the performance of TPB on the bi-objective BBOB function set [8]. We also compare TPB with HMO-CMA-ES and state-of-the-art meta-model-based multi-objective optimizers.

Outline. Section 2 provides some preliminaries. Section 3 reviews related work. Section 4 introduces TPB. Section 5 describes our experimental setting. Section 6 shows analysis results. Section 7 concludes this paper.

Code availability. The code of TPB is available at <https://github.com/royojitanabe/tpb>.

2 PRELIMINARIES

2.1 Multi-objective optimization

We tackle a multi-objective minimization of a vector-valued objective function $f : \mathbb{X} \rightarrow \mathbb{R}^M$, where $\mathbb{X} \subseteq \mathbb{R}^N$ is the search space. Note that M is the dimension of the objective space, and N is the dimension of the search space. Let $f = (f_1, \dots, f_M)$, where $f_m : \mathbb{X} \rightarrow \mathbb{R}$ is called the m -th objective function. The image of f, \mathbb{R}^M in our case, is called the objective space. Throughout of this paper, we consider a box constrained search space, i.e., $\mathbb{X} = [\text{LB}_1, \text{UB}_1] \times \dots \times [\text{LB}_N, \text{UB}_N]$, where LB_n and UB_n are the lower and upper bounds of the n -th coordinate of the search space.

Our objective is to find a finite set of solutions B that approximates the Pareto front $\mathcal{P}(f)$, which is defined as follows:

$$\mathcal{P}(f) = \{f(x) \mid x \in \mathbb{X}, \nexists y \in \mathbb{X} \text{ s.t. } f(y) < f(x)\}, \quad (1)$$

where $a < b$ (for $a, b \in \mathbb{R}^M$) represents the Pareto dominance relation (1 if $a_i \leq b_i$ holds for all $i = 1, \dots, M$ and $a_j < b_j$ holds for some j , and 0 otherwise). A solution x^* is said to a Pareto optimal solution if no solution in \mathbb{X} can dominate x^* . The Pareto optimal solution set X^* is the set of all x^* . The objective is informally stated as to find a set of approximate Pareto optimal solutions that are well-distributed on $\mathcal{P}(f)$. The quality of B is often measured by a quality indicator such as the hypervolume indicator [67].

In this paper, we suppose that we can access the objective function only through an expensive black-box query $f : x \mapsto f(x)$. Its indication is summarized below. (1) The Jacobian and higher order information of f is unavailable (*derivative-free optimization*). (2) The characteristic constants of f such as the Lipschitz constant are unavailable (*black-box optimization*). (3) Evaluation of $f(x)$ is computationally expensive (*expensive optimization*). (4) Each objective function value $f_m(x)$ cannot be obtained with a lower computational cost. Therefore, the cost of the optimization process is measured by the number of f -calls. We assume that it is limited up to $20 \times N, \dots, 40 \times N$.

2.2 Simplicial problem

Kobayashi et al. [43] defined a class of multi-objective optimization problems whose Pareto optimal solution set and Pareto front can be seen topologically as a simplex. Let M be a positive integer. The *standard* $(M-1)$ -simplex is denoted by

$$\Delta^{M-1} = \left\{ (t_1, \dots, t_M) \in \mathbb{R}^M \mid \sum_{m=1}^M t_m = 1, t_m \geq 0 \right\}.$$

Let $I := \{1, \dots, M\}$ be the index set on the objective functions. For each non-empty subset $J \subseteq I$, we define

$$\Delta^J := \{(t_1, \dots, t_M) \in \Delta^{M-1} \mid t_m = 0 \ (m \notin J)\}$$

and

$$f_J := (f_j)_{j \in J} : \mathbb{X} \rightarrow \mathbb{R}^{|J|}.$$

Definition 2.1. For a given objective function $f : \mathbb{X} \rightarrow \mathbb{R}^M$, the multi-objective optimization problem of minimizing f is *simplicial* if there exists a map $\phi : \Delta^{M-1} \rightarrow \mathbb{X}$ such that for each non-empty subset $J \subseteq I$, its restriction $\phi|_{\Delta^J} : \Delta^J \rightarrow \mathbb{X}$ gives the following homeomorphisms:

$$\phi|_{\Delta^J} : \Delta^J \rightarrow X^*(f_J), \quad (2)$$

$$f \circ \phi|_{\Delta^J} : \Delta^J \rightarrow \mathcal{P}(f_J). \quad (3)$$

2.3 Bézier simplex fitting

We denote the set of non-negative integers (including zero) by \mathbb{N} . Let D be an arbitrary integer in \mathbb{N} , and

$$\mathbb{N}_D^M := \left\{ (d_1, \dots, d_M) \in \mathbb{N}^M \mid \sum_{m=1}^M d_m = D \right\}.$$

An $(M-1)$ -Bézier simplex of degree D is a mapping $\mathbf{b} : \Delta^{M-1} \rightarrow \mathbb{R}^N$ determined by control points $\mathbf{p}_d \in \mathbb{R}^N$ ($\mathbf{d} \in \mathbb{N}_D^M$) as follows:

$$\mathbf{b}(t) := \sum_{\mathbf{d} \in \mathbb{N}_D^M} \binom{D}{\mathbf{d}} t^{\mathbf{d}} \mathbf{p}_d, \quad (4)$$

where $\binom{D}{\mathbf{d}} := \frac{D!}{d_1! \dots d_M!} (\in \mathbb{R})$ is a multinomial coefficient, and $t^{\mathbf{d}} := t_1^{d_1} \dots t_M^{d_M} (\in \mathbb{R})$ is a monomial for each $\mathbf{t} := (t_1, \dots, t_M) \in \Delta^{M-1}$ and $\mathbf{d} := (d_1, \dots, d_M) \in \mathbb{N}_D^M$. The following theorem ensures that the Pareto optimal solution set and Pareto front of any simplicial problem can be approximated with arbitrary accuracy by a Bézier simplex of an appropriate degree:

THEOREM 2.2 (Kobayashi *ET AL.* [43, THEOREM 1]). *Let $\phi : \Delta^{M-1} \rightarrow \mathbb{R}^N$ be a continuous map. There is an infinite sequence of Bézier simplices $\mathbf{b}^{(i)} : \Delta^{M-1} \rightarrow \mathbb{R}^N$ such that*

$$\lim_{i \rightarrow \infty} \sup_{\mathbf{t} \in \Delta^{M-1}} \|\phi(\mathbf{t}) - \mathbf{b}^{(i)}(\mathbf{t})\| = 0.$$

With this result, Kobayashi *et al.* [43] proposed the Bézier simplex fitting method to describe the Pareto optimal solution set of a simplicial problem. Suppose that we have a set of approximate Pareto optimal solutions $\{(\mathbf{x}_l, \mathbf{t}_l) \in \mathbb{X} \times \Delta^{M-1} \mid l = 1, \dots, L\}$, where \mathbf{x}_l and \mathbf{t}_l are the l -th approximate Pareto optimal solution and its corresponding parameter, respectively. The Bézier simplex fitting method adjusts the control points by minimizing the ordinary least squares (OLS) loss function: $\frac{1}{L} \sum_{l=1}^L \|\mathbf{x}_l - \mathbf{b}(\mathbf{t}_l)\|^2$. Since the OLS loss function is a convex quadratic function with respect to \mathbf{p}_d , its minimization problem can be solved efficiently, for example, by solving a normal equation.

3 RELATED WORK

Two-phase approaches have been well studied in the context of multi-objective optimization (e.g., [28, 36, 37, 54]). TPLS+PLS [21, 50] is one of the most representative two-phase approaches for combinatorial optimization. Roughly speaking, the first phase in multi-objective two-phase approaches aims to find well-converged solutions to the Pareto front. Then, the second phase aims to generate a set of well-diversified solutions based on the solutions obtained in the first phase. Generally, two-phase approaches can produce only a poor-quality solution set when it stops before the maximum

budget of function evaluations [20]. Thus, the anytime performance of most two-phase approaches is poor. Here, we say that the anytime performance of an optimizer is good if it can obtain a well-approximated solution set at any time during the search process. The substantial difference between TPB and existing two-phase approaches is that the second phase in TPB incorporates solutions by utilizing a Bézier simplex model, which fully exploits the theoretical property of the Pareto optimal solution set. In addition, unlike TPB, all two-phase approaches but [54] were designed for non-expensive optimization. Here, the study [54] proposed a surrogate model-based approach for constrained bi-objective optimization.

Some methods for interpolating objective vectors (not solutions) obtained by an EMO algorithm have been proposed in the literature [5, 34, 35]. A decision-maker can determine her/his preference by visually examining interpolated objective vectors. One of the most representative approaches is the PAINT method [35], which interpolates an objective vector set using the Delaunay triangulation. Note that these interpolation methods cannot provide an inverse mapping from the objective space to the search space. In contrast, the second phase in TPB aims to interpolate solutions (not objective vectors) to approximate the Pareto front.

The Pareto estimation method [24] aims to increase the number of non-dominated solutions obtained by an EMO algorithm. The Pareto estimation method uses a neural network model to find an inverse mapping from the objective space to the search space. GAN-LMEF [63] interpolates randomly generated solutions on the manifold by using dimensionality reduction, clustering, and GAN [25]. These two methods aim to interpolate a sufficiently large number of solutions. In contrast, the second phase in TPB aims to interpolate only K solutions (i.e., $K = M + 1 = 2 + 1 = 3$ in this study) by utilizing a Bézier simplex model.

Some EMO algorithms (e.g., RM-MEDA [66]) exploit the simplex structure of the Pareto optimal solution set. BeZEA [46] evolves a control point set for a Bézier curve to generate a high-quality solution set in terms of the “smoothness” measure, which was proposed in [46]. Unlike these EMO algorithms, TPB exploits the property of the Pareto optimal solution set by using the theoretically well-founded Bézier simplex. No previous study also proposed an EMO algorithm based on the simplex structure of the Pareto optimal solution set for computationally expensive optimization.

4 PROPOSED FRAMEWORK

This section describes the proposed TPB, which consists of the first phase (Section 4.1) and the second phase (Section 4.2). Let $\mathbf{W} = \{\mathbf{w}_k\}_{k=1}^K$ be a set of K weight vectors. We assume that $K = M + 1$, which is the minimum value of K .

In the first phase (Section 4.1), TPB aims to approximate K Pareto optimal solutions by applying a single-objective optimizer to K scalar optimization problems $\{g_{\mathbf{w}_k}\}_{k=1}^K$. Let \mathbf{B}^* be a set of the best K solutions for the K scalar problems obtained in the first phase. Here, the k -th solution in \mathbf{B}^* should correspond to the k -th weight vector in \mathbf{W} . Ideally, the first phase should find \mathbf{B}^* such that \mathbf{x}_k in \mathbf{B}^* minimizes its corresponding scalar problem $g_{\mathbf{w}_k}$. Let budget be the maximum budget of function evaluations for the whole process of TPB. The first phase in TPB can use $\lfloor \text{budget} \times r^{\text{1st}} \rfloor$ function evaluations in the maximum case, where $r^{\text{1st}} \in [0, 1]$ is a control

parameter of TPB. For example, when $\text{budget} = 40$ and $r^{1\text{st}} = 0.9$, 36 function evaluations can be used in the first phase in the maximum case. Note that some optimizers have their own stopping criteria in addition to the maximum number of function evaluations. For example, BOBYQA stops when reaching its minimum trust region radius. Thus, it is possible that the first phase in TPB does not use all $\lfloor \text{budget} \times r^{1\text{st}} \rfloor$ function evaluations.

The second phase in TPB (Section 4.2) aims to interpolate the K solutions in B^* by using a Bézier simplex-based interpolation method [43]. The Bézier simplex model can approximate the Pareto optimal solution set (see Section 2.3). In addition, the Bézier simplex-based interpolation can be done by minimizing the OLS function, which is a convex quadratic function.

Below, Sections 4.1 and 4.2 describe the first and second phases in TPB, respectively. Section 4.3 discusses the property of TPB.

4.1 First phase

Algorithm 1 shows the first phase in TPB. In line 1 in Algorithm 1, $\text{budget}^{\text{opt}}$ is the maximum budget of function evaluations used in an optimizer on each scalar problem. In line 2 in Algorithm 1, X is an archive that maintains all solutions found so far.

As in D-TPLS [50], the first phase in TPB first performs single-objective optimization of each objective function $f \in \{f_1, \dots, f_M\}$ (lines 3–6 in Algorithm 1). This aims to approximate M Pareto optimal solutions that minimize the M objective functions, respectively. Unlike D-TPLS, the M solutions are mainly used for the normalization procedure in the next step (lines 7–15 in Algorithm 1). TPB sets the initial solution \mathbf{x}_{init} to the center of the search space $\mathbf{x}_{\text{center}}$ (line 3 in Algorithm 1), where the n -th element in $\mathbf{x}_{\text{center}}$ is $(\text{LB}_n + \text{UB}_n)/2$. Then, TPB applies a pre-defined single-objective optimizer (`optimizer`) to each objective function (line 5 in Algorithm 1). Here, Y is a set of all solutions found by `optimizer`.

Next, the first phase in TPB aims to solve the remaining $K - M$ scalar problem(s). Since TPB has solved the M objective functions, TPB here does not consider the M extreme weight vectors $\{\mathbf{e}_m\}_{m=1}^M$ (line 7 in Algorithm 1). TPB sets the approximated ideal point $\mathbf{z}^{\text{ideal}} \in \mathbb{R}^M$ and the approximated nadir point $\mathbf{z}^{\text{nadir}} \in \mathbb{R}^M$ based on X (line 8 in Algorithm 1). Note that this step always normalizes the objective vector $\mathbf{f}(\mathbf{x})$ as follows: $\mathbf{f}(\mathbf{x}) = (\mathbf{f}(\mathbf{x}) - \mathbf{z}^{\text{ideal}}) / (\mathbf{z}^{\text{nadir}} - \mathbf{z}^{\text{ideal}})$. The initial solution \mathbf{x}_{init} is set to the best solution in X in terms of a given scalarizing function (line 9 in Algorithm 1).

Finally, we set $B^* = \{\mathbf{x}_{\text{best},k}\}_{k=1}^K$, where $\mathbf{x}_{\text{best},k}$ is the best-so-far solution of the k -th scalar problem (lines 12–15 in Algorithm 1). The second phase in TPB interpolates the K solutions in B^* .

4.2 Second phase

Let $\text{budget}^{1\text{st}}$ be the number of function evaluations used in the first phase, where the maximum budget $^{1\text{st}}$ is $\lfloor \text{budget} \times r^{1\text{st}} \rfloor$. The second phase in TPB uses the remaining $\text{budget}^{2\text{nd}} = \text{budget} - \text{budget}^{1\text{st}}$ function evaluations.

Let $T^{\text{fit}} = \{\mathbf{t}_k^{\text{fit}}\}_{k=1}^K$ be a set of K parameter vectors, where $\mathbf{t}_k^{\text{fit}} \in \Delta^{M-1}$. TPB treats the k -th weight vector \mathbf{w}_k in W as the k -th parameter $\mathbf{t}_k^{\text{fit}}$ in T^{fit} . Thus, T^{fit} is identical to W . With B^* and T^{fit} , we next train a Bézier simplex model $\mathbf{b} : \Delta^{M-1} \rightarrow \mathbb{R}^N$ that takes a parameter $\mathbf{t} \in \Delta^{M-1}$ as an input and outputs a minimizer

Algorithm 1: The first phase in TPB

```

1 budgetopt ← ⌊(budget × r1st)/K⌋;
2 X ← ∅;
3 xinit ← xcenter;
4 for f ∈ {f1, ..., fM} do
5   Y ← Run optimizer on f with xinit and budgetopt;
6   X ← X ∪ Y;
7 for w ∈ W \ {em}_{m=1}^M do
8   Set zideal and znadir based on X;
9   xinit ← argminx ∈ X{gw(x|zideal, znadir)};
10  Y ← Run optimizer on gw with xinit and budgetopt;
11  X ← X ∪ Y;
12 B* ← ∅;
13 for w ∈ W do
14   xbest ← argminx ∈ X{gw(x|zideal, znadir)};
15  B* ← B* ∪ {xbest};
    
```

of the corresponding scalarizing function. Specifically, TPB fits a Bézier simplex model \mathbf{b} to B^* with T^{fit} by solving the OLS loss minimization problem:

$$\text{minimize } \sum_{k=1}^K \|\mathbf{x}_k - \mathbf{b}(\mathbf{t}_k^{\text{fit}})\|^2, \quad (5)$$

where \mathbf{x}_k is the k -th solution in B^* .

Let T^{int} be a set of $\text{budget}^{2\text{nd}}$ parameter vectors. After fitting the Bézier simplex model \mathbf{b} in (5), TPB generates $\text{budget}^{2\text{nd}}$ solutions by using \mathbf{b} and T^{int} . It is expected that the $\text{budget}^{2\text{nd}}$ solutions complement the K solutions in B^* . Any method can be used to generate T^{int} , e.g., uniform random generation. The decision maker's preference can also be incorporated into T^{int} . In this study, we generate $\text{budget}^{2\text{nd}}$ parameters in T^{int} so that they are equally spaced. First, we equally generate $(\text{budget}^{2\text{nd}} + M)$ parameters on Δ^{M-1} . Then, we removed the M extreme parameters (1, 0) and (0, 1) from T^{int} . Since the first phase has found the M extreme solutions, we do not need to re-generate them. For example, when $\text{budget}^{2\text{nd}} = 4$, we can obtain the following parameters: $\mathbf{t}_1^{\text{int}} = (0.2, 0.8)$, $\mathbf{t}_2^{\text{int}} = (0.4, 0.6)$, $\mathbf{t}_3^{\text{int}} = (0.6, 0.4)$, and $\mathbf{t}_4^{\text{int}} = (0.8, 0.2)$.

4.3 Discussion

4.3.1 Control parameters for TPB. The numerical control parameters for TPB include the number of weight vectors K , the degree in a Bézier simplex model D , and the budget ratio $r^{1\text{st}}$. Clearly, the best setting of K and D depends on the shape of the Pareto optimal solution set. We believe that K must be more than or equal to $M + 1$ so that a resulting Bézier simplex model can characterize the shape of the Pareto optimal solution set. This is because a Bézier simplex model fitting needs at least one non-extreme solution to handle the nonlinear Pareto optimal solution set. Similarly, D must be more than or equal to 2 to handle the nonlinearity of the Pareto optimal solution set. The best setting of $r^{1\text{st}}$ depends on the difficulty in

solving K scalar problems. If K scalar problems are easy, r^{1st} should be a small value. Otherwise, the first phase in TPB can waste computational resources. However, as described at the beginning of Section 4, some modern optimizers (e.g., BOBYQA) automatically terminate the search. Thus, we believe that r^{1st} can be set to a relatively high value (e.g., $r^{1st} = 0.9$).

The categorical control parameters for TPB include the scalarizing function g and the single-objective optimizer. Although TPB can use any g (e.g., the weighted Tchebycheff function), we set g to the weighted sum function $g_w^{ws} = \sum_{m=1}^M w_m f_m(x)$ in this study. Since g^{ws} is the simplest scalarizing function, g^{ws} is a reasonable first choice. A mathematical derivative-free optimizer is suitable for optimizer for the reason discussed in Section 1. We set optimizer to BOBYQA, which is a state-of-the-art mathematical derivative-free optimizer for box-constrained optimization. The first phase in HMO-CMA-ES also adopts g^{ws} and BOBYQA.

4.3.2 Advantages and disadvantages of TPB. One advantage of TPB is that it can use a state-of-the-art single-objective optimizer without any change. In contrast to meta-model-based optimizers, TPB does not require computationally expensive operations if a single-objective optimizer is computationally cheap. TPB can also exploit the structure of the Pareto solution set by using the theoretically well-understood Bézier simplex.

As described in Section 3, the anytime performance of two-phase approaches is generally poor. TPB has the same disadvantage. The second phase in TPB cannot interpolate K solutions when a given problem is not simplicial (see Section 2.2). This is because a Bézier simplex model can represent only a standard $(M - 1)$ -simplex. Fortunately, for a lot of practical real-world problems, scatter plots of approximate Pareto optimal solutions imply those problems are simplicial (e.g., [47, 56, 59, 62]).

5 EXPERIMENTAL SETUP

We investigated the performance of the proposed TPB using COCO [32], which is the standard benchmarking platform in the GECCO community. We used the 55 bi-objective BBOB problems (f_1, \dots, f_{55}) [8] provided by COCO. The first and second objective functions in a bi-objective BBOB problem are selected from the 24 single-objective noiseless BBOB functions [33]. Although the DTLZ [19] and WFG [38] problems are the most commonly-used test problems, many previous studies (e.g., [10, 13, 41]) pointed out that they have some serious issues, including the regularity of the Pareto front and the existence of distance and position variables. In contrast, the bi-objective BBOB problems address all these issues. Each bi-objective BBOB problem consists of 15 instances in COCO. A single run of a multi-objective optimizer was performed on each problem instance. In other words, 15 runs were performed for each problem. We set the number of variables N to 2, 3, 5, 10, and 20.

We used an automatic performance indicator (I_{COCO}) [11] provided by COCO. COCO uses an unbounded external archive to maintain all non-dominated solutions found so far. When there exists at least a single solution in the archive that dominates a reference point $(1, 1)^T$ in the normalized objective space $[0, 1]^M$, the performance of optimizers is measured by a referenced version of the hypervolume indicator [67] using the archive. Otherwise, the

performance of optimizers is measured by the smallest distance to the region of interest, which is bounded by the nadir point.

We compare TPB with HMO-CMA-ES [45], ParEGO [42], MOTPE [49], K-RVEA [14], KTA2 [57], and EDN-ARMOEA [26]. We demonstrate the effectiveness of the second phase in TPB by comparing with the warm start phase in HMO-CMA-ES, which is based on a sophisticated scalarizing approach. We are also interested in the performance of TPB compared to state-of-the-art meta-model-based optimizers. We used the optuna [1] implementation of MOTPE and the PlatEMO [60] implementation of the surrogate-assisted EMO algorithms. We used the results of HMO-CMA-ES provided by the COCO data archive (<https://numbbio.github.io/data-archive>).

We set the control parameters for TPB based on the discussion in Section 4.3.1, i.e., $K = M + 1 = 3$ and $D = 2$. We used BOBYQA and g^{ws} as optimizer and g , respectively. Here, we evaluated the performance of TPB with $r^{1st} \in \{0.7, 0.8, 0.9\}$ on the first BBOB problem f_1 with $N = 2$ in our preliminary study. We set r^{1st} to 0.9 based on the rough hand-tuning results. We used the Py-BOBYQA [12] implementation of BOBYQA. Unlike HMO-CMA-ES, we used the default parameter setting of BOBYQA. For the Bézier simplex model fitting method, we used the code provided by the authors of [43] (<https://gitlab.com/hmkz/pytorch-bsf>). We used a workstation with an Intel(R) 48-Core Xeon Platinum 8260 (24-Core \times 2) 2.4GHz and 384GB RAM using Ubuntu 18.04.

We set the maximum budget of function evaluations (budget) to $20 \times N$, $30 \times N$, and $40 \times N$. As discussed in Section 4.3.2, TPB is not an anytime algorithm. Thus, the behavior of TPB depends on the termination condition, i.e., budget in this study. The performance of some state-of-the-art surrogate-assisted EMO algorithms (e.g., K-RVEA and KTA2) also depends on budget. This is because they are not anytime algorithms similar to TPB. For example, K-RVEA has a temperature-like parameter that determines the magnitude of the penalty value. Generally, the best parameter setting for EMO algorithms depends on budget [4, 22]. In addition, budget has not been standardized in the field of computationally expensive multi-objective optimization. For the above-discussed reasons, we used the three budget settings.

6 RESULTS

This section describes our analysis results. Through experiments, Sections 6.1–6.4 address the following research questions.

- **Section 6.1** How does TPB interpolate solutions?
- **Section 6.2** Is TPB competitive with state-of-the-art optimizers?
- **Section 6.3** How important is the two-phase mechanism in TPB?
- **Section 6.4** How does the choice of K and r^{1st} influence the performance of TPB?

6.1 On the solution interpolation in TPB

Figure 1 shows the distribution of solutions generated by TPB for budget = $20 \times N$. Figure 1 shows the results on the first instance of f_1 with $N = 2$. Note that the solution interpolation in TPB is performed in the search space (Figure 1(a)), not the objective space (Figure 1(b)). In Figure 1, we confirmed that budget^{1st} = $0.9 \times 20 \times 2 = 36$ and budget^{2nd} = $40 - 36 = 4$.

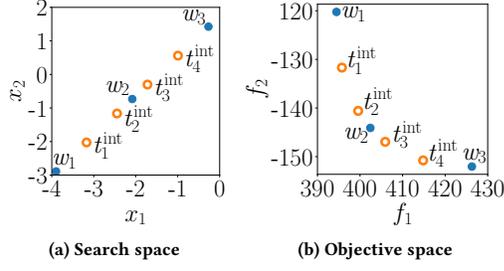


Figure 1: Distribution of solutions obtained by TPB for f_1 for $N = 2$ in the search and objective spaces.

In Figure 1, the three blue filled circles represent the three solutions in B^* found in the first phase with the three weight vectors $w_1 = (1, 0)$, $w_2 = (0.5, 0.5)$, and $w_3 = (0, 1)$. In contrast, the four orange unfilled circles represent the four solutions generated in the second phase with the four parameters $t_1^{\text{int}}, \dots, t_4^{\text{int}}$ that are the same as in the example in Section 4.2.

As shown in Figure 1, the three solutions obtained in the first phase are well-converged to the Pareto front, but they are sparsely distributed. The second phase makes up for this shortcoming. As seen from Figure 1, the four solutions generated in the second phase incorporate the three solutions. The four solutions are distributed as if they were obtained by a scalar optimization approach with the four weight vectors $(0.2, 0.8)$, $(0.4, 0.6)$, $(0.6, 0.4)$, and $(0.8, 0.2)$. As a result, TPB could obtain the seven well-converged and well-distributed solutions. As demonstrated here, the first and second phases in TPB are complementary to each other.

6.2 Comparison with state-of-the-art optimizers

Figure 2 shows the results of TPB and the six optimizers on the 55 bi-objective BBOB problems with $N \in \{2, 5, 10, 20\}$ and budget $\in \{20 \times N, 30 \times N, 40 \times N\}$. Recall that budget is the maximum budget of function evaluations. We do not show the results for $N = 3$, but they are similar to the results for $N = 2$. Most meta-model-based optimizers require extremely high computational cost, especially for higher dimensions and larger budgets. Experiments on the 825 ($= 55 \times 15$) BBOB instances for each dimension is also time-consuming. For these reasons, we stopped an optimizer when it did not finish within a week. The missing results in Figure 2 indicate that the corresponding optimizer was stopped before reaching budget, e.g., the results of KTA2 for $N = 10$ in Figure 2(c). In Figures 2, “best 2016” shows the performance of a *virtual* best solver constructed based on the results of 15 optimizers participating in the GECCO BBOB 2016 workshop. Thus, “best 2016” does not mean the best actual optimizer. The cross in Figure 2 shows the number of function evaluations used in each optimizer. Since ParEGO, K-RVEA, KTA2, and EDN-ARMOEA cannot stop exactly at a pre-defined budget, their crosses exceed budget in some cases, e.g., the results of KTA2 for $N = 2$ in Figure 2(a).

Figure 2 shows the bootstrapped empirical cumulative distribution (ECDF) [10, 30] based on the results on all 55 bi-objective BBOB problems. We used the COCO postprocessing tool cocopp with the

expensive option `-expensive` to generate all ECDF figures in this paper. For each problem instance, let I^{ref} be the I_{COCO} indicator value of the Pareto optimal solution set. Let also $I^{\text{target}} = I^{\text{ref}} + \epsilon$ be a target value to reach, where ϵ is any one of 31 precision levels $\{0.5, \dots, 50\}$ in the expensive setting. Thus, 31 I^{target} values are available for each problem instance. The vertical axis in the ECDF figure represents the proportion of I_{COCO} values reached by the corresponding optimizer within specified function evaluations. Here, the horizontal axis represents the number of function evaluations. For example, Figure 2(d) indicates that HMO-CMA-ES solved about 60 % of the 31 I^{target} values within $10 \times N$ evaluations for $N = 20$.

Statistical significance is tested with the rank-sum test for a given I^{target} value by using COCO. Due to space limitation, we show the results in the supplementary material. Note that the statistical test results are generally consistent with the results in Figure 2.

As shown in Figure 2, HMO-CMA-ES is the clear winner within $10 \times N$ function evaluations for any N . The five meta-model-based optimizers perform almost the same until $11 \times N - 1$ function evaluations. This is because they generate the initial solution set of size $11 \times N - 1$ by Latin hypercube sampling. These results suggest that scalarization-based approaches with BOBYQA as in HMO-CMA-ES perform the best when only a very small number of function evaluations (i.e., $10 \times N$ evaluations) are available.

Some meta-model-based optimizers (e.g., ParEGO and K-RVEA) perform better than HMO-CMA-ES for more than $11 \times N - 1$ evaluations, especially for larger budgets. We observed that the ranks of some meta-model-based optimizers depend on the maximum budget. For example, for $N = 5$, as shown in Figure 2(b), KTA2 performs the worst when budget $= 20 \times N$. In contrast, as shown in Figure 2(f), KTA2 performs the best at the end of the run when budget $= 30 \times N$. These observations indicate that the performance of some meta-model-based optimizers is sensitive to budget. One may wonder about the high performance of ParEGO. We believe that this is due to the performance evaluation based on the unbounded external archive. Although an analysis of the performance of meta-model-based optimizers is beyond the scope of this paper, it is an interesting research direction.

As seen from Figures 2(a), (e), and (i), TPB performs poorly compared to the state-of-the-art optimizers for $N = 2$. In contrast, TPB achieves a good performance at the end of the run for $N = 5$. As shown in Figures 2(c), (d), (g), (h), (k), and (l), TPB is the best performer at the end of the run for $N = 10$ and $N = 20$. These results indicate the effectiveness of TPB for budget $= 20 \times N$, $30 \times N$, and $40 \times N$ for $N \geq 10$.

Figure 3 shows the average computation time of each optimizer over the 15 instances of f_1 for budget $= 20 \times N$. We expect that the computation time of HMO-CMA-ES is the same or less than that of TPB. We could not measure the computation time of ParEGO, KTA2, and EDN-ARMOEA for $N = 20$ in practical time due to their high computational cost. As seen from Figure 3, the computation time of TPB is lower than those of the five meta-model-based optimizers, except for the results of MOTPE for $N \leq 3$. The computation of TPB took approximately 6.6 seconds even for $N = 20$. These results indicate that TPB is faster than meta-model-based optimizers in terms of computation time.

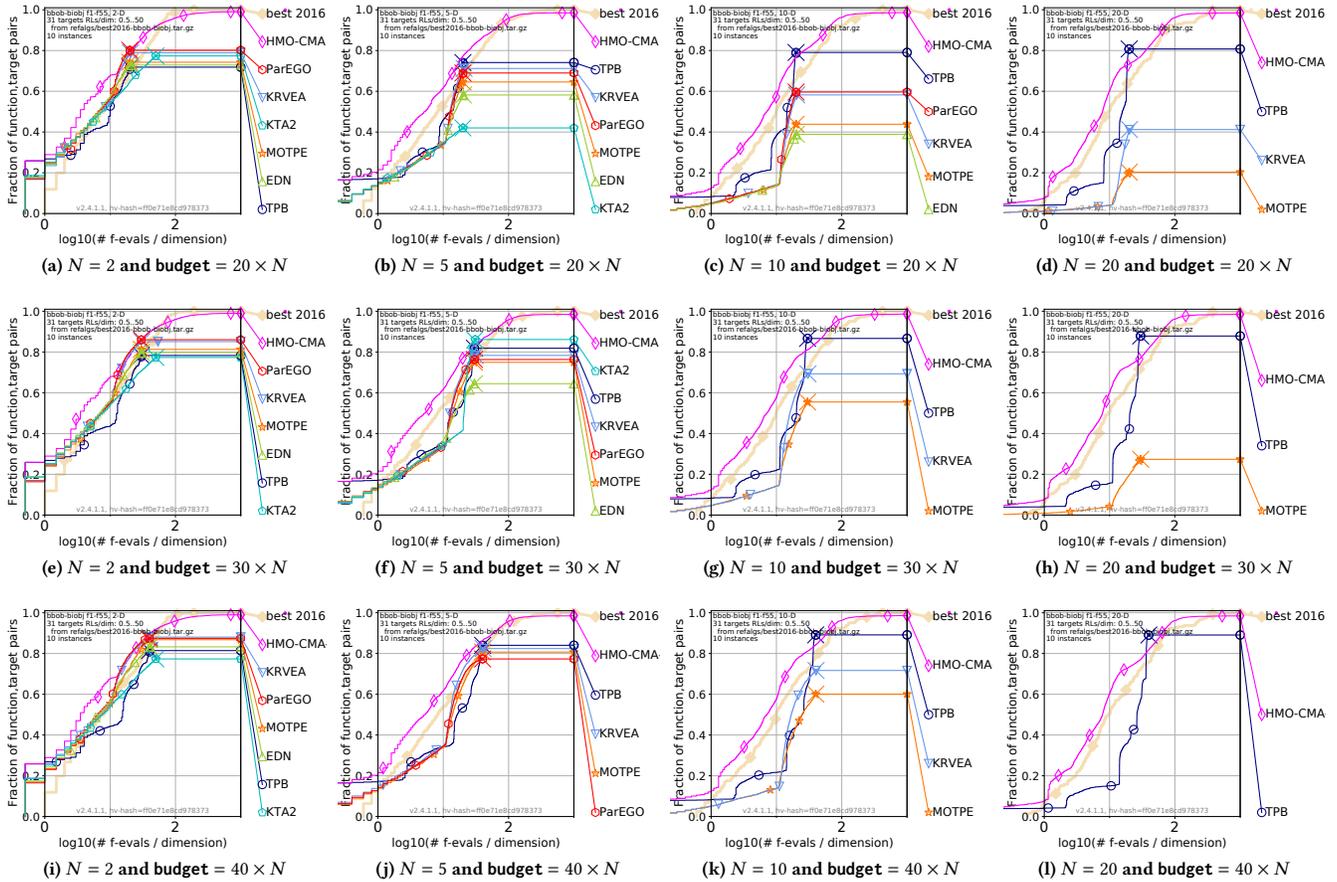


Figure 2: Comparison with state-of-the-art optimizers. “HMO-CMA” and “EDN” stand for HMO-CMA-ES and EDN-ARMOEA, respectively.

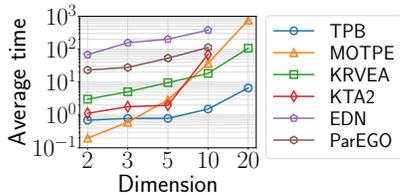


Figure 3: Average computation time (sec) of each optimizer over the 15 instances of f_1 for budget = $20 \times N$.

Figure 4 shows the results on f_1 , f_{28} , f_{46} , and f_{53} , which are the multi-objective versions of the Sphere, Rosenbrock, (rotated) Rastrigin, and (rotated) Schwefel functions. As discussed in Section 4.3, the Bézier simplex model-based interpolation method assumes that a given problem is simplicial. Although an in-depth theoretical analysis is needed, we believe that the 15 unimodal (and weakly-multimodal) bi-objective BBOB problems satisfy the assumption, including f_1 and f_{28} . As shown in Figures 4(a) and (b), TPB obtains a good performance on f_1 and f_{28} . The results on other unimodal problems (except for f_{11} , f_{12} , and f_{20}) are relatively similar to Figures

4(a) and (b). In contrast, the remaining 40 multi-modal bi-objective BBOB problems do not satisfy the assumption, including f_{46} and f_{53} . As seen from Figure 4(c), the poor performance of TPB on f_{46} is consistent with our intuition. However, Figure 4(d) shows that TPB unexpectedly performs the best on f_{53} . Similar results were observed on other ten multimodal problems (e.g., f_9 and f_{10}). These results suggest that the solution interpolation method can possibly perform well even when a given problem is not simplicial. A further investigation is needed in future research.

In summary, we demonstrated the effectiveness of TPB for computationally expensive multi-objective optimization. Our results on the bi-objective BBOB problems show that TPB performs better than HMO-CMA-ES and meta-model-based optimizers for $N \geq 10$. We also observed that TPB is computationally cheaper than meta-model-based optimizers for $N \geq 5$.

6.3 Importance of the two-phase mechanism

Here, let us consider the first phase-only TPB (TPB1) and the second phase-only TPB (TPB2). We investigate the importance of the two-phase mechanism in TPB by comparing it with TPB1 and TPB2. While TPB1 does not perform the second phase, TPB2 does not

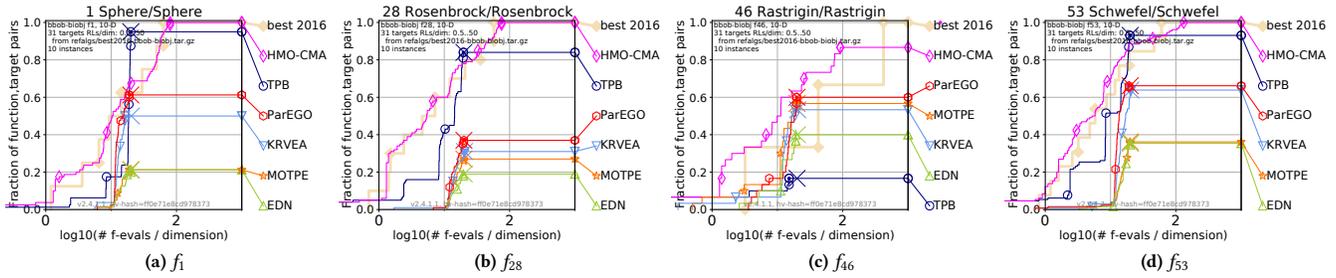


Figure 4: Comparison with state-of-the-art optimizers on four selected problems with $N = 10$ (budget = $20 \times N$).

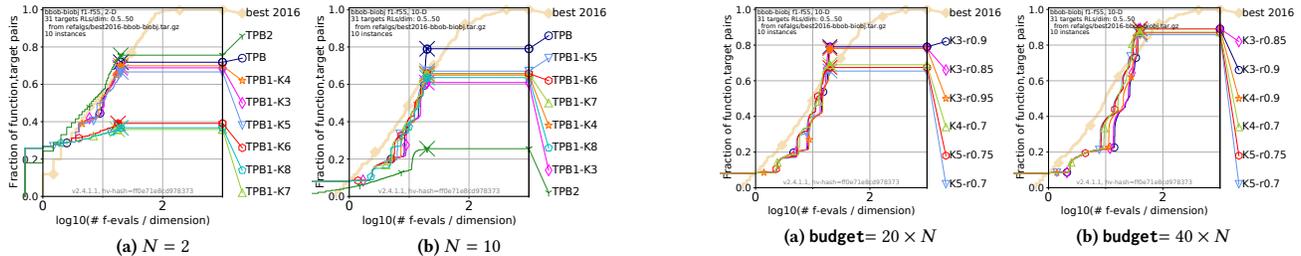


Figure 5: Comparison of TPB, TPB1, and TPB2.

Figure 6: Comparison of TPB with various K and r^{1st} .

perform the first phase. First, as in most meta-model-based optimizers (e.g., K-RVEA), TPB2 generates the initial solution set of size $11 \times N - 1$ by Latin hypercube sampling. Then, TPB2 performs the second phase based on the best K out of the $11 \times N - 1$ solutions.

Figure 5 shows the comparison of TPB, TPB1, and TPB2 on the 55 bi-objective BBOB problems with $N = 2$ and 10 for budget = $20 \times N$. Note that the results for $N \in \{3, 5, 20\}$ are similar to the results for $N = 10$. The results show that TPB1 performs worse than TPB at the end of the run for $N = 2$ and 10. Interestingly, as shown in Figure 5(a), TPB2 outperforms TPB for $N = 2$. We observed that TPB2 performs well on multimodal problems for $N = 2$. However, as seen from Figure 5(b), TPB2 performs significantly poorly for $N = 10$. These results demonstrate the effectiveness of the two-phase mechanism in TPB.

6.4 Impact of K and r^{1st}

Although Section 4.3.1 gave the default values of K and r^{1st} , it is important to understand their impact on the performance of TPB. Figure 6 shows the results of TPB with $K \in \{3, 4, 5\}$ and $r^{1st} \in \{0.7, 0.75, 0.8, 0.85, 0.9, 0.95\}$ on the 55 bi-objective BBOB problems for $N = 10$, where budget = $20 \times N$ and $40 \times N$. For example, “K3-r0.9” represents the results of TPB with $K = 3$ and $r^{1st} = 0.9$. For the sake of clarity, Figure 6 shows only the results of TPB with the three best parameter settings and the three worst parameter settings.

As seen from Figure 6(a), the best performance of TPB for budget = $20 \times N$ is obtained when using $K = 3$ and $r^{1st} = 0.9$. In contrast, as shown in Figure 6(b), TPB with $K = 3$ and $r^{1st} = 0.85$ performs the best for budget = $40 \times N$. Figure 6 shows that the gap between the best and worst performance of TPB is relatively small for budget

= $40 \times N$. Although we do not show detailed results here, we observed that the best setting of K and r^{1st} depends on a problem, N , and budget. These results suggest that the performance of TPB can be further improved by tuning the K and r^{1st} values. However, $K = 3$ and $r^{1st} = 0.9$ can be a good first choice for $M = 2$.

7 CONCLUSION

We have proposed TPB for computationally expensive multi-objective black-box optimization. The first phase in TPB fully exploits an efficient derivative-free optimizer to find well-approximated solutions of K scalar problems with a small budget of function evaluations, where $K = M + 1$. The second phase in TPB interpolates the K solutions by the Bézier simplex model-based method that exploits the property of the Pareto optimal solution set. Our results show that TPB performs significantly better than HMO-CMA-ES and some state-of-the-art meta-model-based multi-objective optimizers on the bi-objective BBOB problems with $N \geq 10$ when the maximum budget of function evaluations is set to $20 \times N$, $30 \times N$, and $40 \times N$. We have also investigated the property of TPB.

We believe that TPB gives a new perspective on the field of computationally expensive multi-objective optimization. Although the EMO community has mainly focused on meta-model-based approaches for computationally expensive optimization, TPB provides a new research direction. It may also be interesting to extend TPB to preference-based multi-objective optimization.

ACKNOWLEDGMENTS

This work was supported by JSPS KAKENHI Grant Number 21K17824. We thank Dr. Ilya Loshchilov for providing the code of HMO-CMA-ES.

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