A Particle Filter based Multi-Objective Optimization Algorithm: PFOPS

Bin Liu Member, IEEE, Yaochu Jin Fellow, IEEE

Abstract—This paper is concerned with a recently developed paradigm for population-based optimization, termed particle filter optimization (PFO). This paradigm is attractive in terms of coherence in theory and easiness in mathematical analysis and interpretation. Current PFO algorithms only work for single-objective optimization cases, while many real-life problems involve multiple objectives to be optimized simultaneously. To this end, we make an effort to extend the scope of application of the PFO paradigm to multi-objective optimization (MOO) cases. An idea called path sampling is adopted within the PFO scheme to balance the different objectives to be optimized. The resulting algorithm is thus termed PFO with Path Sampling (PFOPS). The validity of the presented algorithm is assessed based on three benchmark MOO experiments, in which the shapes of the Pareto fronts are convex, concave and discontinuous, respectively.

Index Terms—particle filtering, path sampling, multi-objective optimization, derivative-free optimization, Pareto front.

I. INTRODUCTION

This paper presents a novel MOO algorithm based on the particle filter (PF). The PFO methods belong to the class of population-based derivative-free optimization methods [1–5]. Different from the meta-heuristics based evolutionary computation (EC) methods [6–8], the PFO paradigm is developed based on Bayesian statistics instead of meta-heuristics. As a class of Sequential Monte Carlo (SMC) methods, the convergence of PF under mild conditions has been proved [9]. This result also holds for the PFO methods. In contrast, the class of EC methods is weak in theory due to the lack of a strict and coherent mathematical foundation.

Current PFO methods only work for single-objective optimization (SOO) problems, while many real-life problems involve multiple objectives to be optimized simultaneously. To this end, we make an effort to extend the scope of application of PFO to multi-objective cases. The key insight adopted here is that, if we can construct a series of target distributions that can balance the multiple objectives and make the degree of this balance controllable, then by simulating these distributions via SMC, we can evaluate the Pareto optimal solutions based on the samples yielded from simulations of these target distributions. We borrow an idea called path sampling to construct the target distributions. We show that the resulting method can handle multiple objectives in an elegant and easy-to-implement way while maintaining the theoretical soundness of the PFO framework. Note that the idea of path sampling is originally developed for estimating the marginal likelihoods of candidate models in the context of Bayesian model comparison [10].

The remainder of this paper is organized as follows. Section II briefly introduces the necessary background on MOO problems. Section III describes the proposed algorithm and discusses the relationships between it and the other related works. Section IV presents the simulation results, and finally, Section V concludes.

II. BACKGROUND ON MOO

Let us consider an optimization problem with $M$ objectives as follows

$$\min F(x) = (f_1(x), f_2(x), \ldots, f_M(x)), \text{ subject to } x \in X,$$

where $f_i : X \to \mathbb{R}$ denotes the $i$th real-valued continuous objective function to be minimized, $x = (x_1, \ldots, x_d)$ is a $d$ dimensional decision vector with value space $X$. The difficulty in resolving (1) results from the conflicts among the objectives $f_1, \ldots, f_M$, which means that a decision that decreases the value of $f_m, m \in \{1, \ldots, M\}$ may increase that of $f_n, n \neq m, n \in \{1, \ldots, M\}$. As a consequence, there is no single decision that minimizes all the objectives simultaneously. A basic idea to deal with this conflict is to find a set of optimal decisions that trade-off among these different objectives, which motivates the concept of Pareto dominance.

Given two decisions $x, x' \in X$, we say $x$ (Pareto) dominates $x'$, denoted by $x \prec x'$, iff $f_m(x) \leq f_m(x')$ for all $m \in \{1, \ldots, M\}$ and $\exists m \in \{1, \ldots, M\}$, $f_m(x) < f_m(x')$. A decision $x^* \in X$ is called (globally) Pareto optimal if there is no $x \in X$ such that $x \prec x^*$. The set of all the Pareto optimal decisions is called the Pareto set ($PS$). The set of all Pareto optimal objective vectors, $PF = \{y \in \mathbb{R}^m | y = F(x), x \in PS\}$, is called the Pareto front [11]. Most existent solutions for such MOO problems are based on EC methods, see details in [12–14]. Here we propose an alternative algorithm based on Bayesian statistics in what follows.

III. PFOPS: THE PROPOSED ALGORITHM

Here we adopt a Bayesian probabilistic viewpoint to investigate the optimization problem. According to this viewpoint, our belief on the minimizer $x^*$ of an objective function $f$ can be quantitatively measured by a probability density function (pdf), say $\pi \propto \exp(-f_m)$. If we can simulate $\pi$ by continuously drawing random samples from it, then $x^*$ can be evaluated based on the samples yielded from that simulation. We can improve this viewpoint by borrowing the idea of simulated annealing (SA) via designing a series of target pdfs that asymptotically converge to the set of global
optima. Then, through simulating the target pdfs by e.g., Markov Chain Monte Carlo (MCMC) as in SA [15] or SMC as in [3, 5], one can get a set of random samples whose empirical distribution also converge asymptotically to the set of global optima. Thus the global optima can be evaluated based on the yielded samples. The above discussion is only limited to SOO problems. Now we extend it to the context of MOO.

A. The details of the algorithm

As mentioned in Section II, the problem of MOO can be formulated as a task of searching a set of Pareto optimal decisions, each of which corresponds to a certain degree of tradeoff among the objectives to be optimized. The basic insight adopted here is that, if we can build up a series of proxy target pdfs, each corresponding to a specific amount of balance among the objectives to be optimized, then, by simulating these proxy pdfs one by one, we can estimate the Pareto optimal decisions along with the corresponding Pareto optima. Then, through simulating the target pdfs by e.g., importance weighting: for ∀i, set

\[ ω_i^k = \begin{cases} \pi_k(x^i), & \text{if } k = 1; \\
π_k(x^i)/π_k(x^i), & \text{otherwise.}
\end{cases} \]

Normalize the importance weights: for ∀i, set

\[ ω_i^k = \frac{ω_i^k}{\sum_{i=1}^N ω_i^k}, \]

Resampling: generate N i.i.d. samples \( x^i \sim \text{Unif}(X) \), for ∀i. Initialize \( PS \) as an empty set;

for \( k = 1, \ldots, K \) do

Find \( j = \max_{i \in \{1, \ldots, N\}} \pi_k(x^i) \) and set \( x^i_0 = x^j \);

Importance weighting: for ∀i, set

\[ ω_i^k = \frac{π_k(x^i)}{∑_{i=1}^N π_k(x^i)}, \]

Resampling: generate N i.i.d. samples \( x^i \sim \text{Unif}(X) \), for ∀i. Initialize \( PS \) as an empty set;

Componentwise Metropolis sampling:

for \( j = 1, \ldots, d \) do

Set \( x^j = x^j \), where \( x^j ≜ (x_1^j, \ldots, x_d^j) \);

Modify the \( j \)th dimension of \( x^j \) by setting \( x_1^j \sim N(\cdot|\mu, Σ) \). If \( π_k(x^j) > π_k(x_1^j) \), set \( x_1^j = x^j \);

Calculate acceptance probability

\[ ρ = \min \left\{ \frac{π_k(x^i)}{π_k(x^i)}, 1 \right\}. \]

Accept

\[ x^i = \begin{cases} x^j, & \text{with probability } ρ; \\
x^i, & \text{with probability } 1 − ρ.
\end{cases} \]

Record \( x^i \) into \( PS \);

Set \( PF = \{y \in \mathbb{R}^m \mid y = F(x), x \in PS\} \);

Remove any \( y \in PS \) (if it exists) that satisfies \( ∃x \in PS, x \sim y \) from \( PS \). Then update \( PF \) correspondingly;

Output \( PS \) and \( PF \) as the estimated Pareto set and Pareto front, respectively.

Algorithm 1: The proposed MOO algorithm: PFOPS. In this table, \( x^i_k \) denotes the \( k \)th Pareto optimal decision generated, “Unif” uniform distribution, \( N \) the sample size of \( PF, N(\cdot|\mu, Σ) \) normal distribution with mean \( \mu \) and variance \( Σ, δ(\cdot) \) the delta-mass function located at 0, “∼” means “distributed as”, ∀i is an abbreviation of \( ∃i \in \{1, \ldots, N\} \).
B. Related work

The probabilistic nature of our method makes it closely related with the class of estimation of distribution algorithms (EDAs) [20–22]. They both use probabilistic models to lead the search towards a more promising area in the decision space. The parametric model used in EDAs needs to be fitted and updated in each iteration, while each model fitting operation brings an additional optimization task to be resolved. By contrast, the proposed algorithm here totally frees the user from the issue of repeated model fitting, since the probabilistic models, i.e., the target pdfs here, are precisely defined beforehand and thus do not need to be fit.

The present work also has connections to a class of algorithms called Bayesian optimization (BO) [23, 24], since they are both Bayesian methods used for dealing with optimization problems. The underpinning assumption in these BO methods is that the objective function is too expensive to be evaluated. A basic operation to reduce the number of expensive function evaluations, which also characterizes the BO methods, is to repeatedly fit a model such as the Gaussian process to approximate the objective function based on a growing number of real function evaluations that have been done. By contrast, the proposed PFOPS algorithm is a kind of population-based methods that do not take an assumption of expensive objective function evaluations. Meanwhile, it has no operations of model fitting included.

Finally, the proposed algorithm is surely related with the other existent PFO methods in e.g. [1–5]. In short, the present work can be seen as an extension of existing PFO methods targeting the MOO problem.

IV. PERFORMANCE EVALUATION

We assessed the behavior of the proposed PFOPS algorithm via numerical experiments. We used one celebrated EC based MOO algorithm, NSGA-II [13], as a benchmark of performance comparison. We considered three two-objective optimization problems, in which the shapes of the Pareto fronts are convex, concave and discontinuous, respectively.

A. Convex Pareto Front Case

In this case, we set \( \mathbf{x} = (x_1, x_2) \), \( f_1(\mathbf{x}) \triangleq x_1^2 + x_2^2 \), \( f_2(\mathbf{x}) \triangleq (x_1 - 5)^2 + (x_2 - 5)^2 \), \( x_1 \in [-5, 10] \) and \( x_2 \in [-5, 10] \). For both PFOPS and NSGA-II, we use two parameter settings, called sufficient-sampling and undersampling here, to initialize them. In the sufficient-sampling setting, we allocate for the algorithm enough iterations to run and a much bigger population size for use, in order to check its performance limit. In contrast, the undersampling setting means a limited number of iterations and a far smaller population size allocated. By doing so, we hope we can generalize results observed here to high dimensional cases for which the undersampling setting is the only choice.

Specifically, we set \( K = N = 100 \) in the oversampling setting of PFOPS; and set \( K = 20 \) and \( N = 5 \) in the undersampling setting. In both settings, the value of \( \lambda_k \) in Eqn.(3) is equal-interval sampled between 0 and 1, and the optional step is not executed. For NSGA-II, we use \( \#\text{pop} \) and \( \#\text{Gen} \) to denote its population size and the number of generations, respectively. In the oversampling setting \( \#\text{pop}=100 \) and \( \#\text{Gen}=100 \), while for the undersampling case, \( \#\text{pop}=20 \) and \( \#\text{Gen}=5 \). Now we let \( \#f \) denote the number of fitness evaluations, then we have \( \#f=2 \times K \times N \) for PFOPS and \( \#f=2 \times \#\text{pop} \times \#\text{Gen} \) for NSGA-II. Then we can see that, in both settings, the computational burden for each algorithm (in terms of \( \#f \)) is maintained at the same level. A direct wall clock running time comparison is also listed in Table I, which re-confirms that a fair comparison is made here.

![Fig. 1: The Pareto fronts yielded by PFOPS and NSGA-II. \#pop and \#Gen are hyperparameters of NSGA-II representing the population size and the number of generations, respectively.](image)

We do experiments by running each algorithm under both of the sufficient-sampling and undersampling settings. An illustration of the estimated Pareto fronts obtained from a typical experiment is presented in Fig.1. It shows that, under the sufficient-sampling setting, the Pareto fronts of PFOPS and NSGA-II almost coincide with each other. It indicates that PFOPS will perform as well as NSGA-II under the sufficient-sampling setting if the Pareto front is convex. Fig.1 also shows that, under the undersampling setting, PFOPS performs better than NSGA-II, as the deviation between samples given by PFOPS and the true Pareto front is significantly smaller than that of NSGA-II. Note that here the so-called true Pareto front is exactly an estimate of it given by PFOPS and NSGA-II under the sufficient-sampling setting.

B. Concave and Discontinuous Pareto Front Cases

The aim of the experiment presented here is to test whether the proposed PFOPS algorithm is capable of handling MOO problems that own a non-convex or a discontinuous Pareto front. For such problems, the weighted-sum type trade-off between the objectives, as shown in Eqn.(3), does not work, as its associated function curve is convex and continuous. Hence, an alternative design of \( \pi_k(\mathbf{x}) \) is employed here, which is shown as follows:

\[
\pi_k(\mathbf{x}) = \exp(- \max\{|1 - \lambda_k| f_1(\mathbf{x}) - z_1^*|, \lambda_k| f_2(\mathbf{x}) - z_2^*|\}), \quad (4)
\]
where \( z_1 < \min f_1, z_2 < \min f_2 \), and \( z^* = (z_1^*, z_2^*) \) is termed Utopian point. We consider here two benchmark test functions for MOO, i.e., a 2-dimensional Fonseca-Fleming function [25] defined as follows

\[
\begin{align*}
  f_1(x) &= 1 - \exp\left[-\sum_{i=1}^{2}(x_i - 1/\sqrt{2})^2\right], \\
  f_2(x) &= 1 - \exp\left[-\sum_{i=1}^{2}(x_i + 1/\sqrt{2})^2\right],
\end{align*}
\]

where \(-4 \leq x_i \leq 4, i = 1, 2\), and the Kursawe function [26] defined as follows

\[
\begin{align*}
  f_1(x) &= \sum_{i=1}^{2}[-10 \exp(-0.2 \sqrt{x_i^2 + x_i^2})] \\
  f_2(x) &= \sum_{i=1}^{3}[x_i^{0.8} + 5 \sin(x_i^3)],
\end{align*}
\]

where \(-5 \leq x_i \leq 5, 1 \leq i \leq 3\).

MOO algorithm called PFOPS. This algorithm discriminates itself with the other related works by adopting a path sampling based mechanism to balance the differing objectives within the PFO paradigm. Experimental results show that it performs better than NSGA-II for the considered convex Pareto front case based on the undersampling setting and its performance is comparable to NSGA-II in the other two cases, in which the shape of the Pareto front is concave and discontinuous, respectively.

The present work represents an initial attempt to formulate the MOO problem as a state filtering task and then to handle it using state filtering methods like PF here. This filtering perspective has already been explored in developing PF based SOO algorithms, such as in [1–5]. Combining these previous studies with the present work here, we can see a big picture, in which a unified PFO framework has been built up, which can handle both SOO and MOO problems in a consistent way. The basic operation included in this framework consists of two parts. The first is to construct a series of target pdfs and the second is to sample from the constructed pdfs. This framework is different from the meta-heuristics based EC methods. Compared with EC methods, this framework is theoretically attractive thanks to its probabilistic nature that makes it own a stronger tie to mathematics especially statistics.

Finally, we point out two interesting future works following this line of research. One is to explore efficient mechanisms to construct the target pdfs for problems with more than two objectives and the other is to improve the present algorithm by adopting the simulated annealing strategy.

|                | sufficient-sampling case | undersampling case |
|----------------|--------------------------|-------------------|
| PFOPS          | 5.4951                   | 0.1158            |
| NSGA-II        | 5.2153                   | 0.4171            |

Fig. 2: The estimated Pareto fronts by PFOPS and NSGA-II for an MOO problem which uses the 2D Fonseca-Fleming function as the test function. This case is characterized by a concave Pareto front as shown in the Figure.

Fig. 3: The estimated Pareto fronts by PFOPS and NSGA-II for an MOO problem which uses the Kursawe function as the test function. This case is characterized by a discontinuous Pareto front as shown in the Figure.

V. CONCLUDING REMARKS

In this paper, we extended the scope of application of the PFO paradigm to MOO cases by proposing a novel PF based
REFERENCES

[1] E. Zhou, M.C. Fu, and S.I. Marcus, “A particle filtering framework for randomized optimization algorithms,” in Proc. of the 40th Conf. on Winter Simulation, 2008, pp. 647–654.

[2] P. Stinis, “Stochastic global optimization as a filtering problem,” Journal of Computational Physics, vol. 231, no. 4, pp. 2002–2014, 2012.

[3] B. Liu, “Posterior exploration based Sequential Monte Carlo for global optimization,” Journal of Global Optimization, vol. 69, no. 4, pp. 847–868, 2017.

[4] B. Liu, S. Cheng, and Y. Shi, “Particle filter optimization: A brief introduction,” in Int’l Conf. in Swarm Intelligence. Springer, 2016, pp. 95–104.

[5] E. Zhou and X. Chen, “Sequential Monte Carlo simulated annealing,” Journal of Global Optimization, vol. 55, no. 1, pp. 101–124, 2013.

[6] J. Kennedy, “Particle swarm optimization,” in Encyclopedia of Machine Learning, pp. 760–766. Springer, 2011.

[7] M. Mitchell, An introduction to genetic algorithms, MIT press, 1998.

[8] M. Dorigo and C. Blum, “Ant colony optimization theory: A survey,” Theoretical Computer Science, vol. 344, no. 2-3, pp. 243–278, 2005.

[9] N. Chopin, “Central limit theorem for Sequential Monte Carlo methods and its application to Bayesian inference,” The Annals of Statistics, vol. 32, no. 6, pp. 2385–2411, 2004.

[10] A. Gelman and X. Meng, “Simulating normalizing constants: From importance sampling to bridge sampling to path sampling,” Statistical Science, pp. 163–185, 1998.

[11] K. Deb, “Multi-objective optimization,” in Search methodologies, pp. 403–449. Springer, 2014.

[12] Q. Zhang and H. Li, “MOEA/D: A multiobjective evolutionary algorithm based on decomposition,” IEEE Trans. on Evolutionary Computation, vol. 11, no. 6, pp. 712–731, 2007.

[13] K. Deb, A. Pratap, S. Agarwal, and T. Meyarivan, “A fast and elitist multiobjective genetic algorithm: NSGA-II,” IEEE Trans. on Evolutionary Computation, vol. 6, no. 2, pp. 182–197, 2002.

[14] R.T. Marler and J.S. Arora, “Survey of multi-objective optimization methods for engineering,” Structural and Multidisciplinary Optimization, vol. 26, no. 6, pp. 369–395, 2004.

[15] S. Kirkpatrick, C.D. Gelatt, and M.P. Vecchi, “Optimization by simulated annealing,” Science, vol. 220, no. 4598, pp. 671–680, 1983.

[16] M. S. Arulampalam, S. Maskell, N. Gordon, and T. Clapp, “A tutorial on particle filters for online nonlinear/non-Gaussian Bayesian tracking,” IEEE Trans. on Signal Processing, vol. 50, no. 2, pp. 174–188, 2002.

[17] A. Doucet, S. Godsill, and C. Andrieu, “On Sequential Monte Carlo sampling methods for Bayesian filtering,” Statistics and Computing, vol. 10, no. 3, pp. 197–208, 2000.

[18] J.S. Liu and R. Chen, “Sequential Monte Carlo methods for dynamic systems,” Journal of the American Statistical Association, vol. 93, no. 443, pp. 1032–1044, 1998.

[19] H. Haario, E. Saksman, and J. Tamminen, “Componentwise adaptation for high dimensional MCMC,” Computational Statistics, vol. 20, no. 2, pp. 265–273, 2005.

[20] B. Liu, S. Cheng, and Y. Shi, “Improving estimation of distribution algorithms with heavy-tailed student’s t distributions,” in 2018 Tenth Int’l Conf. on Advanced Computational Intelligence (ICACI). IEEE, 2018, pp. 11–16.

[21] V.A. Shim, K.C. Tan, and C.Y. Cheong, “A hybrid estimation of distribution algorithm with decomposition for solving the multiobjective multiple traveling salesman problem,” IEEE Trans. on Systems, Man, and Cybernetics, Part C (Applications and Reviews), vol. 42, no. 5, pp. 682–691, 2012.

[22] H. Karshenas, R. Santana, C. Bieza, and P. Larrañaga, “Multiobjective estimation of distribution algorithm based on joint modeling of objectives and variables,” IEEE Trans. on Evolutionary Computation, vol. 18, no. 4, pp. 519–542, 2014.

[23] B. Shahriari, K. Swersky, Z. Wang, R.P. Adams, and N. De Freitas, “Taking the human out of the loop: A review of bayesian optimization,” Proceedings of the IEEE, vol. 104, no. 1, pp. 148–175, 2016.

[24] D. Hernández-Lobato, J. Hernández-Lobato, A. Shah, and R. Adams, “Predictive entropy search for multi-objective bayesian optimization,” in Int’l Conf. on Machine Learning (ICML), 2016, pp. 1492–1501.

[25] C.M. Fonseca and P.J. Fleming, “An overview of evolutionary algorithms in multiobjective optimization,” Evolutionary Computation, vol. 3, no. 1, pp. 1–16, 1995.

[26] F. Kursawe, “A variant of evolution strategies for vector optimization,” in Int’l Conf. on Parallel Problem Solving from Nature. Springer, 1990, pp. 193–197.