ZOOpt: Toolbox for Derivative-Free Optimization

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Abstract

Recent advances of derivative-free optimization allow efficient approximating the global optimal solutions of sophisticated functions, such as functions with many local optima, non-differentiable and non-continuous functions. This article describes the ZOOpt¹ toolbox that provides efficient derivative-free solvers and are designed easy to use. ZOOpt provides a Python package for single-thread optimization, and a light-weighted distributed version with the help of the Julia language for Python described functions. ZOOpt toolbox particularly focuses on optimization problems in machine learning, addressing high-dimensional, noisy, and large-scale problems. The toolbox is being maintained toward ready-to-use tool in real-world machine learning tasks.

Keywords: Software, Derivative-free optimization, Hyper-parameter optimization, Non-convex optimization, Subset selection, Distributed optimization

1. Derivative-Free Optimization

Optimization, e.g., $x^* = \operatorname{argmin}_{\boldsymbol{x} \in \mathcal{X}} f(\boldsymbol{x})$ as a general representative, is fundamental in machine learning. Derivative-free optimization, also termed as zeroth-order or black-box optimization, involves a kind of optimization algorithms that does not rely on gradient information. It only relies on the function values $f(\boldsymbol{x})$ on the sampled solution \boldsymbol{x} . Representative algorithms include evolutionary algorithms (Hansen et al., 2003), Bayesian optimization (Shahriari et al., 2016), optimistic optimization (Munos, 2014), model-based optimization (Yu et al., 2016), etc.

Since the conditions of applying derivative-free algorithms are quite few, they are suitable for tackling sophisticated optimization tasks (e.g., with many local optima, non-differentiable, non-continuous). Thus, derivative-free optimization has achieved remarkable applications in machine learning, including hyper-parameter optimization (Thornton et al., 2013; Feurer et al., 2015), direct policy search (Salimans et al., 2017; Hu et al., 2017), subset selection (Qian et al., 2015), image classification (Real et al., 2017), etc.

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^{1.} https://github.com/eyounx/ZOOpt

Some open-source packages of derivative-free optimization approaches have been available, including individual algorithms such as CMA-ES² (Hansen et al., 2003), SMAC³ (Hutter et al., 2011), IMGPO⁴ (Kawaguchi et al., 2015), and RACOS⁵ (Yu et al., 2016); packages of a kind of algorithms such as DEAP⁶ (Fortin et al., 2012), BayesOpt⁷ (Martinez-Cantin, 2014), and Spearmint⁸ (Snoek et al., 2011); and those particularly designed for hyper-parameter optimization with machine learning frameworks, such as Scikit-Optimize⁹ and Hyperopt¹⁰ (Bergstra et al., 2011). These packages either provide general-purpose tools, or tools for a specific task (i.e., hyper-parameter tuning) in learning. The design of the ZOOpt aims at building a ready-to-use tool for solving more generic optimization problems in machine learning, which require high efficiency, scaling-up, noise-handling, etc.

2. Methods in ZOOpt

With the aim of supporting machine learning tasks, ZOOpt includes a set of methods that are efficient and performance-guaranteed, with add-ons handling noise and high-dimensionality.

Optimization in continuous space. We implement SRACOS (Hu et al., 2017) as the default optimization method for continuous space, which has shown high efficiency in a range of learning tasks. Optional method is RACOS (Yu et al., 2016), a batch version of SRACOS. A routine is in place to setup the default parameters of the two methods, while users can override them.

Optimization in discrete space. Both SRACOS and RACOS can also be applied to discrete space. However, if the optimization task is in a binary vector space with constraints, such as the subset selection problem, POSS (Qian et al., 2015) is the default optimization method, which has been proven with the best-so-far approximation quality on these problems.

Noise handling. Noise has a great impact on the performance of derivative-free optimization. Resampling is the most straightforward method to handle noise, which evaluates one sample several times to obtain a stable mean value. Besides resampling, more efficient methods including value suppression (Wang et al., 2018) and threshold selection (Qian et al., 2017) are implemented.

High-dimensionality handling. Increase of the search space dimensionality badly injures the performance of derivative-free optimization. When a high dimensional search space has a low effective-dimension, random embedding (Wang et al., 2016) is an effective way to improve the efficiency. Also, the sequential random embeddings (Qian et al., 2016) can be used when there is no clear low effective-dimension.

^{2.} https://www.lri.fr/~hansen/cmaes_inmatlab.html

^{3.} http://www.cs.ubc.ca/labs/beta/Projects/SMAC/

^{4.} http://lis.csail.mit.edu/code/imgpo.html

^{5.} https://github.com/eyounx/RACOS

^{6.} https://github.com/deap/deap

^{7.} https://bitbucket.org/rmcantin/bayesopt/

^{8.} https://github.com/JasperSnoek/spearmint

^{9.} https://github.com/scikit-optimize/scikit-optimize

^{10.} http://jaberg.github.io/hyperopt/

3. Structure of ZOOpt

Single-thread optimization. ZOOpt single-thread version is implemented purely in Python, which provides easy integrality with other machine learning frameworks in Python. ZOOpt itself is an independent package and can also be installed from PyPI using pip.

In ZOOpt, an optimization problem is abstracted in several components: Objective, Dimension, Parameter, and Solution, where each is a Python class. An Objective object is initialized with a function and a Dimension object as the input, where the Dimension object defines the dimension size and boundaries of the search space. A Parameter object specifies algorithm parameters. ZOOpt is able to automatically choose parameters for a range of problems, leaving only one parameter of the optimization budget (i.e. the number of solution evaluations) needed to be manually determined according to the time of the user. The Opt .min function make the optimization happen, and will return a Solution object which contains the final solution and the function value. Moreover, after the optimization, the Objective object contains the history of the optimization for observation. Although ZOOpt is purly in Python, we have made a lot effort to improve the efficiency of the code. Several concrete examples and full functions are available at the Github. **Distributed optimization**. To utilize many cores and many machines, ZOOpt has a light-weighted distributed version, utilizing the network structure in Figure 1. Evaluation servers are used to calculate function values of given solutions. Evaluation servers start up by registering to the control server. When a client comes with a task, it first retrieves evaluation servers from the control server, and sends the evaluation requests to the evaluation servers. This structure aims at easing the manager of evaluation servers for multiple clients.

Due to the advance of parallel performance of Julia language, ZOOpt implements the core codes of the client in Julia. However, the evaluation servers and the control server are implemented in Python, which means the objective function provided by the user to ZOOpt is still described in Python. Also, the evaluation process, running at the evaluation server end, can utilize the full environments in Python.

To fully utilize the distributed computing environment, Distributed ZOOpt employs the asynchronous variant of the optimization algorithm. We test the performance of Distributed ZOOpt optimizing the Ackley function with many local minima. In order to simulate CPU-bound tasks, one million ex-

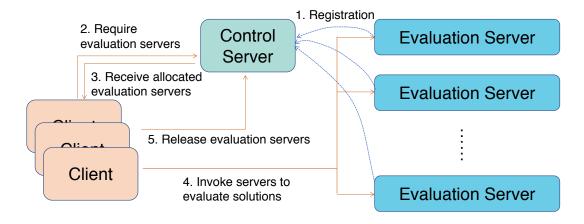


Figure 1: Distributed ZOOpt structure and process for distributed optimization.

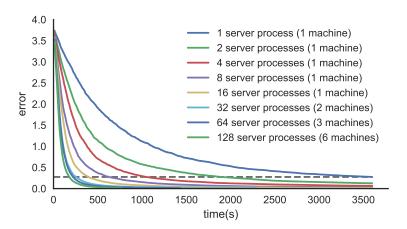


Figure 2: An evaluation of Distributed ZOOpt for optimizing Ackley function with extra delay.

tra for loops are added to extend evaluation time in each evaluation of the Ackley function. The budget is set to 100 thousand, and the time limit is one hour. Results on different number of evaluation server processes are shown in Figure 2. It can be observed that that Distributed ZOOpt can make well use of more than 100 processes across multiple machines. More examples and detailed instructions are available in the Github website.

Acknowledgments

We would like to acknowledge support for this project from National Key Research and Development Program (2017YFB1001903), and Jiangsu Science Foundation (BK20170013).

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