Bayesian Optimization with Local Search

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Abstract. Global optimization finds applications in a wide range of real world problems. The multi-start methods are a popular class of global optimization techniques, which are based on the ideas of conducting local searches at multiple starting points, and then sequentially determine the starting points according to some prescribed rules. In this work we propose a new multi-start algorithm where the starting points are determined in a Bayesian optimization framework. Specifically, the method can be understood as to construct a new function by conducting local searches of the original objective function, where the new function attains the same global optima as the original one. Bayesian optimization is then applied to find the global optima of the new local search based function.

1 Introduction

Global optimization (GO) is a subject of tremendous potential applications, and has been an active research topic since. There are several difficulties associated with solving a global optimization problem: the objective function may be expensive to evaluate and/or subject to random noise, it may be a black-box model and the gradient information is not available, and the problem may admit a very large number of local minima, etc. In this work we focus on the last issue: namely, in many practical global optimization problems, it is often possible to find a local minimum efficiently, especially when the gradient information of the objective function is available, while the main challenge is to escape from a local minimum and find the global solution. Many metaheuristic GO methods, such simulated annealing \cite{11} and genetic algorithm \cite{4}, can avoid being trapped by a local minimal, but these methods do not take advantage of the property that a local problem can be quite efficiently solved, which makes them less efficient in the type of problems mentioned above.

A more effective strategy for solving such problems is to combine global and local searches, and the multi-start (MS) algorithms \cite{12} have become a very popular class of methods along this line. Loosely speaking the MS algorithms attempt to find a global solution by performing local optimization from multiple starting points. Compared to search based global optimization algorithms, the (MS) methods combine the local and the global searches, which makes it particularly suitable for problems where a local optimization can be performed efficiently. The most popular MS methods include the clustering \cite{8, 19} and the Multi Level Single Linkage (MDSL) \cite{15} methods and the OptQuest/NLP algorithm \cite{20}. More recently, new MS algorithms have been proposed and applied to machine learning problems \cite{5, 10}. One of the most important issues in a MS algorithm is how to determine the initial points, i.e. the points to start a local search (LS) from. Most MS algorithms determine the initial points sequentially, which in each step requires to find the next initial point based on the current information. We shall adopt this setup in this work and so the question we want to address in the present work is how to determine the next “best” initial point given the information at the current step.

The main idea presented in this work is to sequentially determine the starting points in a Bayesian optimization (BO) \cite{17, 18, 14} framework. The standard BO algorithm is designed to solve a global optimization problem directly without using LS: it uses a Bayesian framework and an experimental design strategy to search for the global minimizers: it builds a probabilistic surrogate model of the objective function using a Gaussian process regression, and then use an acquisition function to determine where to query the objective function. The BO algorithms have found success in many practical GO problems, especially for those expensive and noisy objective functions \cite{3}. Nevertheless, the BO methods do not take advantage of efficient local solvers even when that is possible. In this work, instead of applying BO directly to the global optimization problem, we propose to use it to identify starting points for the local solvers in a MS formulation. Within the BO framework, we can determine for the starting points using a rigorous and effective experimental design approach.

An alternative view of the proposed method is that we define a new function by solving a local optimization problem of the original objective function. By design the newly defined function is discrete-valued and has the same global optimizers as the original objective function. And we then perform BO to find the global minima for the new function. From this perspective, the method can be understood as to pair the BO method with a local search, and we restate that the method requires that the local problems can be solved efficiently. For example, in many statistical learning problems with large amounts of data, an estimate of the gradients can be computed more efficiently than the evaluation of the objective function \cite{1}, and it follows that a local solution can be obtained efficiently. The rest of the work is organized as follows. In Section\textsuperscript{2} we introduce the MS algorithms for GO problems, and present our BO based method to identify the starting points. In Section\textsuperscript{3} we provide several examples to demonstrate the performance of the proposed method. Finally Section\textsuperscript{4} offers some closing remarks.

2 Bayesian optimization with local search

2.1 Generic multi-start algorithms

Suppose we want to solve a bound constrained optimization problem:

\begin{equation}
\min_{x \in \Omega} f(x),
\end{equation}

where \( \Omega \) is a compact subspace of \( \mathbb{R}^n \). In general, the problem may admit multiple local minimizers and we want to find the global solution of it. As has been mentioned earlier, the MS algorithms are a
class of GO methods for problems where LS can be conducted efficiently. The MS iteration consists of two steps: a global step where a initial point is generated, and a local step which performs a local search from the generated initial point. A pseudocode of the generic MS algorithm is given in Alg. 1. It can be seen here that one of the key issues of the MS algorithm is how to generate the starting point in each iteration. A variety of methods have been proposed to choose the starting points, and they are usually designed for different type of problems. For example, certain methods such as assume that the evaluation of the objective function is much less computationally expensive than the local searches, and as a result they try to reduce the number of local searches at the price of conducting a rather large number of function evaluations in the state space. On the other hand, in another class of problems, a satisfactory local solution may be obtained with a reasonable computational cost, and as will be discussed later we shall use the BO algorithm to determine the initial points. For that purpose, we next give a brief overview of BO.

Algorithm 2 The BO algorithm
1: generate a number of points \( \{x_1, \ldots, x_{N_0}\} \) in \( \Omega \);
2: evaluate \( y_n = f(x_n) \) for \( n = 1 : N_0 \);
3: let \( D_{N_0} = \{ (x_n, y_n) \}_{n=1}^{N_0} \);
4: construct a GP model from \( D_{N_0} \), denoted as \( \hat{f}_{N_0} \);
5: \( n = N_0 \);
6: while stopping criteria are not satisfied do
7: \( x_{n+1} = \arg \max \alpha(x; \hat{f}_n) \)
8: \( y_{n+1} = f(x_{n+1}) \);
9: augment data \( D_{n+1} = D_n \cup \{ (x_{n+1}, y_{n+1}) \} \);
10: update GP model obtaining \( \hat{f}_{n+1} \);
11: \( n = n + 1 \);
12: end while
13: return \( y_{\text{min}} = \min \{ y_n \}_{n=1}^{N} \);

where \( f(\cdot) \) is the objective function, \( x \) is the initial point of the local search, and \( x^* \) is the obtained local minimal point. \( L \) can represent any local optimization approach, with or without gradient, and we require that for any given initial point \( x^* \), the solver \( L \) will return a unique local minimum \( x^* \). Using both \( L \) and \( F \), we can define a new function
\[
y = F_L(x) = f(x^*),
\]
where \( x^* \) is the output of Eq. (2) with objective function \( f \) and initial point \( x \). That is, the new function \( F_L \) takes a starting point \( x \) as its input, and returns the local minimal value of \( f \) found by the local solver \( L \) as its output. It should be clear that \( F_L \) is a well-defined function on \( R^n \), which has the same global minima as function \( f(x) \). Moreover, suppose that \( f(x) \) only has a finite number of local minima, and \( F_L(x) \) is discrete-valued. Please see Fig. 1 for a schematic illustration of the new function defined by LS and its GP approximation. Next we apply standard BO algorithm to the newly constructed function \( F_L(x) \), and the global solution of \( F_L \) found by BO is regarded as the global solution of \( f(x) \). We refer to the proposed algorithm as BO with LS (BOwLS) and we provide the complete procedure of it in Alg. 3. We restate that, as one can see from the algorithm, BOwLS is essentially a MS algorithm, which uses the BO experimental design criterion to determine the next starting point. When desired, multiple starting points can also be determined in the BO framework, and we refer to the aforementioned BO references for details of this matter.

Algorithm 3 The BOwLS algorithm
1: let \( D_0 = \emptyset \);
2: for \( n = 1 : N_0 \) do
3: solve \( [y^*, x^*] = L(f(x), x_n) \);
4: let \( y_n = y^* \);
5: augment data \( D_n = D_{n-1} \cup \{ (x_n, y_n) \} \)
6: end for
7: construct a GP model from \( D_{N_0} \), denoted as \( \hat{f}_{N_0} \);
8: \( n = N_0 \);
9: while stopping criteria are not satisfied do
10: \( x_{n+1} = \arg \max \alpha(x; \hat{f}_n) \)
11: solve \( [y^*, x^*] = L(f(x), x_{n+1}) \);
12: let \( y_{n+1} = y^* \);
13: augment data \( D_{n+1} = D_n \cup \{ (x_{n+1}, y_{n+1}) \} \);
14: update GP model obtaining \( f_{n+1} \);
15: \( n = n + 1 \);
16: end while
17: return \( y_{\text{min}} = \min \{ y_n \}_{n=1}^{N} \);

2.2 Bayesian Optimization
The Bayesian optimization (BO) is very popular global optimization method, which treats the objective function as a blackbox. Simply put, BO involves the use of a probabilistic model that defines a distribution over objective function. In practice the probabilistic model is usually constructed with the Gaussian Process (GP) regression: namely the function \( f(x) \) is assumed to be a Gaussian process defined on \( \Omega \), the objective function is queried at certain locations, and the distribution of the function value at any location \( x \), conditional on the observations, which is Gaussian, can be explicitly computed from the Bayesian formula. Please see Appendix A for a brief description of the GP construction. Based on the current GP model of \( f(x) \) the next point to query is determined in an experimental design formulation. Usually the point to query is determined by maximizing an acquisition function \( \alpha(x, f) \) where \( f \) is the GP model of \( f \), which is designed based on the exploration and the exploitation purposes of the algorithm. Commonly used acquisition functions include the Expected Improvement, the Probability of Improvement, and the Upper Confidence Bound, and interested readers may consult [13] for detailed discussions and comparisons of these acquisition functions. We describe the standard version of BO in Alg. 2.

2.3 The BO with LS algorithm
Now we present our method that integrate MS and BO. The idea behind the method is rather simple: we perform BO for a new function which has the same global minima as the original function \( f(x) \). The new function is defined via conducting local search of \( f(x) \). Specifically suppose we have local solver \( L \) defined as,
\[
x^* = L(f(\cdot), x),
\]
3 Numerical examples

In this section, provide several mathematical and practical examples to demonstrate the performance of the proposed method. In each example, we solve the GO problem with three methods: MLSL, the efficient multi-start (EMS) in [5] and the BOwLS method proposed in this work.

3.1 Mathematical test functions

We first consider six mathematical examples that are commonly used as the benchmarks for GO algorithms, selected from [4]. The objective functions, the domains and the global optimal solutions of these functions are provided in Appendix B. As is mentioned earlier, we solve these problems with MLSL, EMS and BOwLS methods, and, since all the algorithm are subject to certain randomness, we repeat the experiments for 50 times. The local search is conducted with the conjugate gradient method using the SciPy package [7]. In these examples we shall assume that evaluating the objective function and its gradient is of similar computational cost, and so we measure the total computational cost by summation of the number of function evaluations and that of the gradient evaluations. For test purpose, we set the stopping criterion to be that the number of function/gradient combined evaluations exceeds 10,000. In our tests, we have found that all the three methods can reach the actual global optima with in the stopping criterion in the first five functions. In Figs. 2 we compare the average numbers of the combined evaluations to reach the global optimal value for all the three methods (the error bars indicate the standard deviations) in the first five functions.

3.2 Gaussian mixture model

A Gaussian mixture model (GMM) can be understood as a parametric model for density estimation. It assumes that the data points are generated from a mixture of a finite number of Gaussian distributions with parameters that need to be estimated from the data. Because of its mixture nature, GMM is often used as a clustering tool and to this end, one can think of mixture models as generalizing k-means clustering to incorporate information about the covariance structure of the data as well as the centers of the latent Gaussian components. Mathematically, a GMM can be written as,

\[ p_{GMM}(x) = \sum_{j=1}^{m} w_j \mathcal{N}(x; \mu_j, \Sigma_j), \]  

subject to \( \sum_{j=1}^{m} w_j = 1 \), where \((\mu, \Sigma)\) is a Gaussian distribution with mean \(\mu\) and covariance \(\Sigma\). It should be clear here that in a GMM, the parameters that need to be determined are the weight \(w_j\), mean \(\mu_j\), and covariance \(\Sigma_j\).
\[ \mu_j \text{ and covariance } \Sigma_j \text{ for each mixture component } (i = 1 \ldots m). \text{ Now suppose that we have a training set } \{x_i\}_{i=1}^n \text{ and the parameters are then determined by maximizing the likelihood function:} \]

\[ \max_{\{w_j, \mu_j, \Sigma_j\}_{j=1}^m} \prod_{i=1}^n p_{GMM}(x_i) = \prod_{i=1}^n \sum_{j=1}^m w_j N(x_i; \mu_j, \Sigma_j), \] 

subject to \( \sum_{j=1}^m w_j = 1 \). Usually this problem is solved with the Expectation Maximization algorithm which can only converge to a local optimum [13]. In this work, we search for the global optimal solution of the problem using the three aforementioned GO algorithms.

In our numerical experiments, we test the methods with two sets of data. The first set of data is generated from a 2-dimensional 3-component GMM, where the three equally weighted components are centered at \([2, 2], [6, 6] \text{ and } [10, 10]\) respectively, all with identity covariance. We draw 210 training data points and 210 test data points.
from the model. We apply the three methods to minimize the negative log-likelihood function of the model. As is in the first example, we repeat the experiments 100 times and we plot the average minimal function value against the number of function/gradient combined evaluations in Fig. 5. We note here that, for this example the performance of the EMS method is significantly worse than the other two methods and so we omit it from the figure. On the other hand, the other two methods yield quite similar performances while that of BOwLS is slightly better. To further evaluate the performances of the methods, we compute the prediction accuracy of the models obtained by the three methods, and the prediction accuracy results averaged over the 100 tests are respectively, 83% (EMS), 85% (MLSL), and 90% (BOwLS). The 2nd dataset is the Iris data, which contains the data for 50 flowers from each of 3 species. The original Iris data contains four attributes, and in this example we use the petal length and width for the clustering problem. The dataset is randomly split into 135 training and 15 test data points. Once again, we repeat the experiments 100 times and we plot the average results of the three methods Fig. 6. One can see from the figure that, the results are qualitatively similar to the first dataset: the results of BOwLS and MLSL are similar while EMS converges considerably slower than the other two. Just like the first dataset, BOwLS has the best performance in all the three methods in this dataset as well. We also compute the average accuracy using the test set, which are 93% (EMS), 97% (MLSL) and 99% (BOwLS) respectively.

3.3 Logistic regression

Finally consider a Logistic regression example. Logistic regression is a common tool for binary regression (or classification). Specifically suppose that we have binary regression problem where the output takes values at \( y = 0 \) or \( y = 1 \), and the probability that \( y = 1 \) is assumed to be the the form of,

\[
h_w(x) = \frac{1}{1 + \exp(-\sum_{i=1}^{m} w_i x_i - w_0)}
\]

where \( x = (x_1, ..., x_m) \) are the predictors and \( w = (w_0, ..., w_m) \) are the coefficients to be determined from data. The cost function for the logistic regression is taken to be

\[
C(h_w(x), y) = \begin{cases} 
- \log(h_w(x)) & \text{if } y = 1 \\
- \log(1 - h_w(x)) & \text{if } y = 0
\end{cases}
\]

Suppose that we have a training set \( \{(x_i, y_i)\}_{i=1}^{n} \), and we then determine the parameters \( w \) by solving the following optimization problem,

\[
\min_{w \in W} \sum_{i=1}^{n} C(h_w(x_i), y_i).
\]

where \( W \) is the domain of \( w \).

In this example we apply the Logistic regression to the Pima Indians Diabetes dataset [16], the goal of which is to diagnose whether a patient has diabetes based on 8 diagnostic measures provided in the data set. The data set contains 768 instances and we split it into a training set of 691 instances and a test set of 77 ones. We solve the result optimization problem (7) with the three GO algorithms, and we repeat the computations for 100 times as before. The minimal function value averaged over the 100 trials is plotted against the number of combined evaluations in Fig. 7. In this example, the EMS method actual performs better than MLSL, while BOwLS has the best performance measured by the number of the function/gradient combined evaluations. Moreover, in the BOwLS method, we expect that as the iteration approaches to the global optimum, the resulting Logistic model should become better and better. To show this, we plot in Fig. 8 the prediction accuracy of the resulting model as a function of the BO iterations (which is also the number of LS), in six randomly selected trials out of 100. The figure shows that the prediction accuracy varies (overall increases) as the number of LS increases, which is a good evidence that the objective function in this example admits multiple local optima and the global optimum is needed for the optimal prediction accuracy.

4 Conclusions

In summary, we have presented a MS algorithm where the starting points of local searches are determined by a BO framework. A main advantage of the method is that the BO framework allows one to
sequentially determine the next starting points in a rigorous and effective experimental design formation. With several numerical examples, we demonstrate that the proposed BOwLS method has highly competitive performance against many commonly used MS algorithms. A major limitation of BOwLS is that, as it is based on the BO framework, it may have difficulty in dealing with very high dimensional problems. We note however that a number of dimension reduction based approaches [3,9] have been proposed to enable BO for high dimensional problems, and we hope that these approaches can be extended to BOwLS as well. In addition, another problem that we plan to work on in the future to combine the BOwLS framework with the stochastic gradient descent type of algorithms to develop efficient GO algorithms for statistical learning problems.

A Construction of the GP model

Given the data set \( D = \{(x_i, y_i)\}_{i=1}^n \), the GP regression performs a nonparametric regression in a Bayesian framework [21]. The main idea of the GP method is to assume that the data points and the new point \((x, y)\) are from a Gaussian Process defined on \( R^n \), whose mean is \( \mu(x) \) and covariance kernel is \( k(x, x') \). Under the GP model, one can obtain directly the conditional distribution \( \pi(y|x, D) \) that is Gaussian: \( \pi(y|x) = \mathcal{N}(\mu_{GP}, \sigma^2_{GP}) \), where the posterior mean and variance are,

\[
\mu_{GP}(x) = \mu(x) + k(x, X)(k(X, X) + \sigma^2_n I)^{-1}(y - \mu(x)) \\
\sigma^2_{GP} = k(x, x) - k(x, X)(k(X, X) + \sigma^2_n I)^{-1}k(X, x).
\]

Here \( y = [y_1, \ldots, y_n] \), \( X = [x_1, \ldots, x_n] \), \( \sigma^2_n \) is the variance of observation noise, \( I \) is an identity matrix, and the notation \( k(A, B) \) denotes the matrix of the covariance evaluated at all pairs of points in set \( A \) and in set \( B \) using the kernel function \( k(\cdot, \cdot) \). In particular, if the data points are generated according to an underlying function \( f(x) \) (which is the objective function in the BO setting), the distribution \( \pi(y|x) \) then provides a probabilistic characterization of the function \( f(x) \) which can be used to predict the function value of \( f(x) \) as well as quantify the uncertainty in the prediction. In Section 2, we refer to this probabilistic characterization, i.e., the Gaussian distribution \( \pi(y|x) \) as \( \hat{f} \). There are a lot of technical issues of the GP construction, such as how to choose the kernel functions and determine the hyperparameters, are left out of this paper, and for more details of the method, we refer the readers to [21].

B The mathematical test functions

The test functions used in Section 3.1 are:

**Price (2-D):**

\[
f(x) = 1 + \sin^2(x_1) + \sin^2(x_2) - 0.1e^{-x_1^2 - x_2^2}.
\]

**Brann (1-D):**

\[
f(x) = (-1.257 + x_1^2 + 0.5\pi + x_2 - 6)^2 + 10(1 - \frac{5}{\pi}\cos(x_1) + 10).
\]

**Cosine-mixture (4-D):**

\[
f(x) = -0.1\sum_{i=1}^{4}\cos(5\pi x_i) - \sum_{i=1}^{4} x_i^2.
\]

**Trid (6-D):**

\[
f_{TRID}(x) = \sum_{i=1}^{6}(x_i - 1)^2 - \sum_{i=2}^{6} x_ix_{i-1}.
\]

Hartmann (6-D):

\[
f(x) = -\sum_{i=1}^{4}c_i\exp\left(-\sum_{j=1}^{6}a_{ij}(x_j - p_{ij})^2\right),
\]

where

\[
a = \begin{bmatrix}
10.0 & 3.0 & 17.0 & 3.50 & 1.70 & 8.0 \\
0.05 & 10.0 & 17.0 & 0.10 & 8.00 & 14.0 \\
3.0 & 3.50 & 17.0 & 10.0 & 17.0 & 8.0 \\
17.0 & 8.0 & 0.05 & 10.0 & 0.10 & 14.0 \\
0.1312 & 0.1696 & 0.5569 & 0.0124 & 0.8283 & 0.5886 \\
0.2329 & 0.4135 & 0.8307 & 0.3736 & 0.1004 & 0.9991 \\
0.2348 & 0.1451 & 0.3522 & 0.2883 & 0.3047 & 0.6650 \\
0.4047 & 0.8828 & 0.8732 & 0.5743 & 0.1091 & 0.0381
\end{bmatrix},
\]

\[
c = \begin{bmatrix}
1.0 \\
1.2 \\
3.0 \\
3.2 \\
0 \\
0
\end{bmatrix},
\]

\[
p = \begin{bmatrix}
0.1312 & 0.1696 & 0.5569 & 0.0124 & 0.8283 & 0.5886 \\
0.2329 & 0.4135 & 0.8307 & 0.3736 & 0.1004 & 0.9991 \\
0.2348 & 0.1451 & 0.3522 & 0.2883 & 0.3047 & 0.6650 \\
0.4047 & 0.8828 & 0.8732 & 0.5743 & 0.1091 & 0.0381
\end{bmatrix}.
\]

Ackley (n-D):

\[
f(x) = -20e^{-0.2\sqrt{\sum_{i=1}^{n}x_i^2}} - e^{\sum_{i=1}^{n}\cos(2\pi x_i)} + 20 + e,
\]

where \( n \) is taken to be 2 and 4 respectively.

The domains and global minimal values of these functions are shown in Table 1.

| Functions     | domain                     | minimal value |
|---------------|----------------------------|---------------|
| Price         | \([-10, 10]^2\)           | -3            |
| Brann         | \([-4, 10] \times [-16, 16]\) | 0.397          |
| Cosine-mixture 4d | \([-1.1, 1]^d\) | -0.252        |
| Trid          | \([-20, 20]^b\)           | -50           |
| Hartmann      | \([0, 1]^b\)              | -3.233        |
| Ackley        | \([-32.768, -32.768]^b\)  | 0             |

Table 1. The domains and the global minimal values of the test functions.

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REFERENCES

[1] Léon Bottou, ‘Large-scale machine learning with stochastic gradient descent’, in Proceedings of COMPSTAT 2010, 177–186, Springer, (2010).
[2] Eric Brochu, Vlad M Cora, and Nando De Freitas, ‘A tutorial on bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning’, arXiv preprint arXiv:1012.2599, (2010).
[3] Josip Djolonga, Andreas Krause, and Volkan Cevher, ‘High-dimensional gaussian process bandits’, in Advances in Neural Information Processing Systems, pp. 1025–1033, (2013).
[4] Andrea Gavana. ‘Global optimization benchmarks and AMPSO. http://infinity77.net/global_optimization/’. Accessed: 2019-09-30.
[5] András György and Levente Kocsis, ‘Efficient multi-start strategies for local search algorithms’, Journal of Artificial Intelligence Research, 41, 407–444, (2011).
[6] John Henry Holland et al., ‘Adaptation in natural and artificial systems: an introductory analysis with applications to biology, control, and artificial intelligence’, MIT press, 1992.
[7] Eric Jones, Travis Oliphant, Pearu Peterson, et al. SciPy: Open source scientific tools for Python, 2001–.
[8] AHG Rinnooy Kan and Gerrit T Timmer, ‘Stochastic global optimization methods part i: Clustering methods’, Mathematical programming, 39(1), 27–56, (1987).
[9] Kirthevasan Kandasamy, Jeff Schneider, and Barnabás Póczos, ‘High dimensional bayesian optimisation and bandits via additive models’, in International Conference on Machine Learning, pp. 295–304, (2015).
[10] Kenji Kawaguchi, Yu Maruyama, and Xiaoyu Zheng, ‘Global continuous optimization with error bound and fast convergence’, Journal of Artificial Intelligence Research, 56, 153–195, (2016).

[11] Scott Kirkpatrick, C Daniel Gelatt, and Mario P Vecchi, ‘Optimization by simulated annealing’, science, 220(4598), 671–680, (1983).

[12] Rafael Martí, Jose A Lozano, Alexander Mendiburu, and Leticia Hernando, ‘Multi-start methods’, Handbook of Heuristics, 1–21, (2016).

[13] Geoffrey McLachlan and David Peel, Finite mixture models, John Wiley & Sons, 2004.

[14] Jonas Mockus, Bayesian approach to global optimization: theory and applications, volume 37, Springer Science & Business Media, 2012.

[15] A HG Rinnooy Kan and GT Timmer, ‘Stochastic global optimization methods part ii: multi level methods’, Mathematical Programming, 39(1), 57–78, (1987).

[16] Ryan A. Rossi and Nesreen K. Ahmed, ‘The network data repository with interactive graph analytics and visualization’, in AAAI, (2015).

[17] Bobak Shahriari, Kevin Swersky, Ziyu Wang, Ryan P Adams, and Nando De Freitas, ‘Taking the human out of the loop: A review of bayesian optimization’, Proceedings of the IEEE, 104(1), 148–175, (2015).

[18] Jasper Snoek, Hugo Larochelle, and Ryan P Adams, ‘Practical bayesian optimization of machine learning algorithms’, in Advances in neural information processing systems, pp. 2951–2959, (2012).

[19] W Tu and RW Mayne, ‘Studies of multi-start clustering for global optimization’, International journal for numerical methods in engineering, 53(9), 2239–2252, (2002).

[20] Zsolt Ugray, Leon Lasdon, John Plummer, Fred Glover, James Kelly, and Rafael Martí, ‘Scatter search and local nlp solvers: A multistart framework for global optimization’, INFORMS Journal on Computing, 19(3), 328–340, (2007).

[21] Christopher KI Williams and Carl Edward Rasmussen, Gaussian processes for machine learning, MIT Press, 2006.