Towards Dynamic Selection of Evolution Controls in Parallel Bayesian Neural Network-assisted Genetic Algorithm

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1 Introduction

Optimization based on expensive simulation is a tedious task due to the difficulty to obtain insights about the landscape to optimize. To overcome this issue, meta-heuristics are well-suited but require a high number of fitness function evaluations. Parallel computing is a first lever that allows to efficiently evaluate multiple simulation-based solutions. As a complementary way to deal with the expensive computational task, surrogate models are exploited. Surrogate models aim at timely imitating the behavior of the original cost function in timely fashion but provide a lower accuracy. In a surrogate-assisted evolutionary algorithm, the new candidate solutions are either predicted or exactly evaluated according to a criterion called Evolution Control (EC). In this paper we present different ECs and we propose to dynamically select the active EC during the search.

2 Parallel Bayesian Neural Network-assisted Genetic Algorithm

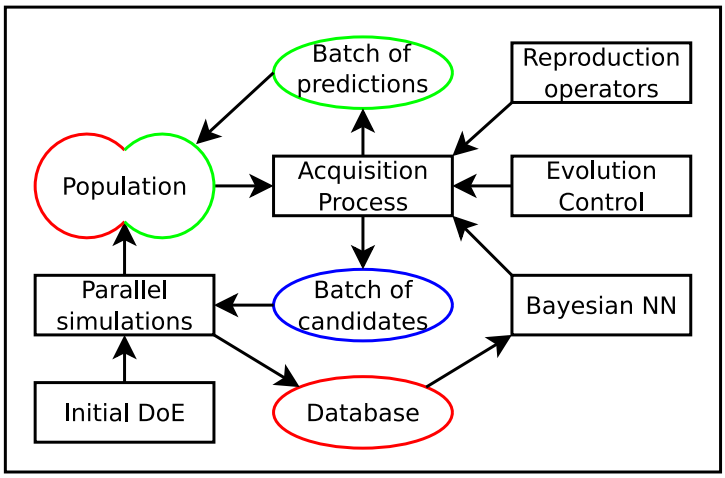

Fig. 1. Structure of Parallel Bayesian Neural Network-assisted Genetic Algorithm. The colored shapes represent sets of solutions. The red shapes are made of simulated solutions, the green shapes are made of predicted solutions and the blue ellipse is made of solutions to be simulated.

In our work, we propose a new parallel surrogate-assisted evolutionary algorithm to deal with expensive black-box optimization problems [1]. This method called Parallel Bayesian Neural Network-assisted Genetic Algorithm (BNN-GA) and whose structure is presented in Fig.1., has been employed with success to solve problems related to tuberculosis transmission control [2].

Multiple candidate solutions are simulated in parallel to take advantage of parallel computing architectures. Indeed, in expensive black-box optimization, other operations such as the Acquisition Process or the surrogate training are negligible. Both to allow parallel simulations and to save the simulation budget limiting the search, batches of solutions are introduced

into the GA. The population is partitioned into batches of parents that are fed into the Acquisition Process. For each batch of parents, the Acquisition Process produces a batch of candidate solutions to be simulated in parallel and a batch of predicted candidate solutions.

After each generation, the best solutions proposed so far are kept to compose the initial population for the next generation. Consequently, the new population possibly embeds predicted solutions. In this configuration, a probable pitfall is that the search may be misled by an inaccurate surrogate. To reduce this risk the EC is employed to decide which solutions can be securely predicted and which ones rather be simulated. To reach this goal, the EC may require uncertainty information about the surrogate prediction. The Monte Carlo Dropout-based Bayesian Neural Network (MCD-BNN) [3] is a surrogate model that, similarly to Gaussian Processes, provides such uncertainty information. The training of MCD-BNN is comparable to that of Artificial Neural Networks and does not suffer from the expensive computational load of fitting Gaussian Processes.

3 Dynamic selection of Evolution Controls

Within the Acquisition Process, reproduction operators are applied on a batch of parents to generate new candidates. The MCD-BNN-aided EC splits the set of candidates into a batch of solutions to be simulated and a batch of predicted solutions. ECs can be classified according to the number of metrics they rely on to make their decision. Let's $\boldsymbol{x}, \boldsymbol{y}$ be two candidate solutions such that one has to be simulated and the other to be predicted. The random no-metric-based EC that selects randomly $\boldsymbol{x}$ or $\boldsymbol{y}$ for simulation is proposed as a baseline in this study.

Let's $\hat{f}()$, $\hat{s}()$ and $d()$ be respectively the surrogate prediction, the surrogate prediction variance and the distance from the database of already simulated solutions. The single-metric-based ECs considered in this study are presented in Table 1. *BP* favours exploitation while *var* and *dist* favours exploration. When the surrogate model does not provide prediction variance, $d()$ can be used as uncertainty information instead.

Name	Description	Criterion
BP	Lowest predicted cost	$\hat{f}(\boldsymbol{x}) < \hat{f}(\boldsymbol{y}) \Rightarrow \boldsymbol{x}$ is simulated
var	Highest prediction variance	$\hat{s}(\boldsymbol{x}) < \hat{s}(\boldsymbol{y}) \Rightarrow \boldsymbol{y}$ is simulated
$dist$	Highest distance from the database	$d(\boldsymbol{x}) < d(\boldsymbol{y}) \Rightarrow \boldsymbol{y}$ is simulated

Table 1. Single-metric-based Evolution Controls.

Two-metrics-based ECs are defined by coupling $\hat{f}()$ with uncertainty information represented either by $\hat{s}()$ or $d()$. The two-metrics-based ECs considered in this study are presented in Table 2. The candidate maximizing the Expected Improvement [4] value proves to be the most promising or uncertain solution. As an alternative to EI, the candidate maximizing the Scaled Expected Improvement [5] value proves to be the most promising or uncertain solution with high confidence. The candidate minimizing the Lower Confidence Bounding [6] proves to be the most promising solution with high confidence. Finally, the candidate showing the best Non Dominated Rank [7] according to the objectives $\hat{f}$ and $-\hat{s}$ or $-d$, when minimization is assumed, should carry the best improvement or uncertainty level and should then be simulated.

Name	Description	Criterion
$EI - var$	Highest Expected Improvement	$EI_{\hat{s}}(\boldsymbol{x}) < EI_{\hat{s}}(\boldsymbol{y}) \Rightarrow \boldsymbol{y}$ is simulated
$EI - dist$		$EI_{d}(\boldsymbol{x}) < EI_{d}(\boldsymbol{y}) \Rightarrow \boldsymbol{y}$ is simulated
$ScaledEI - var$	Highest Scaled Expected Improvement	$ScaledEI_{\hat{s}}(\boldsymbol{x}) < ScaledEI_{\hat{s}}(\boldsymbol{y}) \Rightarrow \boldsymbol{y}$ is simulated
$ScaledEI - dist$		$ScaledEI_{d}(\boldsymbol{x}) < ScaledEI_{d}(\boldsymbol{y}) \Rightarrow \boldsymbol{y}$ is simulated
$LCB - var$	Lowest Lower Confidence Bound	$LCB_{\hat{s}}(\boldsymbol{x}) < LCB_{\hat{s}}(\boldsymbol{y}) \Rightarrow \boldsymbol{x}$ is simulated
$LCB - dist$		$LCB_{d}(\boldsymbol{x}) < LCB_{d}(\boldsymbol{y}) \Rightarrow \boldsymbol{x}$ is simulated
$NDR - var$	Best Non Dominated Rank	$NDR_{(\hat{f},-\hat{s})}(\boldsymbol{x}) < NDR_{(\hat{f},-\hat{s})}(\boldsymbol{y}) \Rightarrow \boldsymbol{x}$ is simulated
$NDR - dist$		$NDR_{(\hat{f},-d)}(\boldsymbol{x}) < NDR_{(\hat{f},-d)}(\boldsymbol{y}) \Rightarrow \boldsymbol{x}$ is simulated

Table 2. Two-metrics-based Evolution Controls.

All the considered ECs offer different trade-offs between exploitation and exploration. Generation by generation, the GA identifies regions from the search space that is considered promising. Since each promising region can present specific characteristics, an appropriate balance between exploitation and exploration should be determined. Under this hypothesis, we propose to study the dynamical adaptation of the current active EC. A system of reward, based on the distance between

the predicted and simulated cost of simulated solutions in the cost space is proposed. At the end of each iteration, the best rewarded EC becomes active. This strategy will be applied to solve problems related to epidemic control.

4 Tuberculosis Transmission Control

Tuberculosis is an airborne disease that has been threatening mankind for thousands of years and still affects around 10 million individuals each year, killing around 1.7 million of them [8]. Previous works suggest that it will be impossible to reach the global elimination targets stated by the World Health Organization with the existing control tools. In this context, main global health agencies and funders increasingly rely on mathematical modeling to design better tuberculosis control policies. Mathematical models such as the AuTuMN model [9] have the ability to simulate transmission within a population and to predict the impact of control interventions on future disease burden.

The problem considered in this paper consists in calibrating a highly stratified version of the AuTuMN model. This model incorporates a high level of complexity since the simulated population can be stratified regarding age, risk factors (diabetes, HIV, smoking...), vaccination status, form of tuberculosis (smear-positive, smear-negative or extrapulmonary) and treatment history [10]. This complexity leads to long computational times and makes the optimization exercise laborious. Model calibration is performed by minimizing a sum-of-square distance between the model predictions and field observations for multiple disease indicators. The 6 calibrated parameters $\{p_i\}_{i\in\{1,\dots,6\}}$ represent the decision variables. If d denotes the calibration sum-of-square distance, the optimization problem is defined by:

$$\min_{p\in\mathbb{R}^6} d(p), \tag{1}$$

$$l_i \leq p_i \leq u_i, \forall i \in \{1, ..., 6\}, \tag{2}$$

where l_i and u_i are the lower and upper bounds associated with parameter p_i, respectively.

5 Conclusion

The availability of parallel computing architectures and the recent advances of machine learning allow to enhance metaheuristics, as proposed by the Parallel BNN-GA method. The emergence of mathematical models simulating tuberculosis transmission allows to formulate expensive black-box optimization problems aiming at decreasing the future disease burden. In this context, the dynamic selection of the Evolution Control within the BNN-GA method is expected to improve the results obtained in past studies when tackling first-rank real-world applications. Extensive experiments are being conducted on Grid'5000 grid platform and the results will be presented at the OLA'20 conference.

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