Surrogate-assisted distributed swarm optimisation for computationally expensive models

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Abstract

Advances in parallel and distributed computing have enabled efficient implementation of distributed swarm and evolutionary algorithms for complex and computationally expensive models. Evolutionary algorithms provide gradient-free optimisation which is beneficial for models that do not have such information available, for instance geoscientific landscape evolution models. However, such models are so computationally expensive that even distributed swarm and evolutionary algorithms with the power of parallel computing struggle. We need to incorporate efficient strategies such as surrogate assisted optimisation that further improves their performance; however this becomes a challenge given parallel processing and inter-process communication for implementing surrogate training and prediction. In this paper, we implement surrogate-based estimation of fitness evaluation in distributed swarm optimisation over a parallel computing architecture. Our results demonstrate very promising results for benchmark functions and geoscientific landscape evolution models. We obtain reduction in computationally time while retaining optimisation solution accuracy though the use of surrogates in a parallel computing environment.

Keywords: Surrogate-assisted optimization, parallel computing, distributed swarm algorithms, landscape evolution models, geoscientific models

1. Introduction

Evolutionary algorithms are loosely motivated by the theory of evolution where species are represented by individuals in a population that compete and collaborate with each other, producing offspring over generations that to improve quality given by fitness measure \cite{1, 2}. Particle swarm optimisation (PSO) on the other hand is motivated by flocking behavior of birds or swarms that is represented by a population of particles (individuals) that compete and collaborate over time \cite{3, 4, 5}. Evolutionary and swarm optimisation methods have been prominent in a number of areas such as real-parameter global optimization, combinatorial optimization and scheduling, and machine learning \cite{6, 7, 8, 9}. Research in evolutionary and swarm optimisation has focused on different ways to create new solutions with mechanisms that are heuristic in nature and hence different variants are available \cite{9, 10}. A major challenge has been in applying them in large scale or computationally expensive optimisation problems that require thousands of function evaluations where a single function evaluation can take minutes to hours or even days \cite{10}. An example of an expensive function is a geo-scientific model for landscape evolution \cite{11}, and deep learning models for big data problems \cite{12}. Computationally expensive optimisation can be addressed with distributed and parallel computing with evolutionary and swarm optimisation \cite{13, 14, 15}; however, we need efficient strategies for representing the problem.

Surrogate assisted optimisation \cite{16, 17, 18, 19} provides a remedy for expensive models with use of statistical and machine learning models to provide a low computational replicate of the actual model. The replica or surrogate is developed by training from available data generated during optimisation that features a set of inputs (new solutions) and corresponding output (fitness) given by actual model. The method is also called Bayesian optimisation where the surrogate model which is known as acquisition function is typically a Gaussian process model \cite{20}; however, neural networks are also used. Evolutionary and swarm optimization methods have been used in surrogate assisted and Bayesian optimization, and been prominent in fields of engine and aerospace design \cite{21, 22, 23, 16}, robotics \cite{20}, experimental design \cite{24}, and machine learning \cite{25, 26}.

Evolutionary algorithms provide gradient-free optimisation which is beneficial for models such as those that do not have expensive models with use of statistical and machine learning models such as those that do not have gradient information, for instance geo-scientific landscape evolution models \cite{27}. Some instances of such models are so expensive that even distributed evolutionary algorithms with the power of parallel computing would struggle. Hence, we need to incorporate efficient strategies such as surrogate assisted optimisation that further improves their performance but this becomes a challenge given parallel processing and inter-process communication for implementing surrogate estimation.

Landscape evolution models are geo-scientific models that has been used to reconstruct the evolution of the Earth’s landscape over millions of years \cite{28, 29, 30}. These models guide geologists and climate scientists in better understanding Earths geologic and climate history that can further also help in foreseeing the distant future of the planet \cite{30, 31}. These mod-
els use data from geological observations such as bore-hole data and estimated landscape topography millions of years ago and require climate conditions and geological parameters that are not easily known. Hence, it becomes an optimisation problem to estimate these parameters which has been tackled mostly with Bayesian inference via Markov Chain Monte Carlo (MCMC) sampling in previous studies that used parallel computing [27], and surrogate assisted Bayesian inference [32]. Motivated by these studies, we bring the problem of landscape evolution model to the evolutionary and swarm optimisation community, rather than viewing it as an inference problem, to see it as an optimisation problem.

In this paper, we implement surrogate-based optimisation framework via swarm optimisation over a parallel computing architecture. We apply the framework for benchmark optimisation functions and a selected landscape evolution model. We investigate performance measures such as accuracy of surrogate prediction given different types of problems, in terms of dimension and fitness landscape.

The rest of the paper is organised as follows. Section 2 provides background and related work, while Section 3 presents the proposed methodology. Section 4 presents experiments and results and Section 5 concludes the paper with discussion for future research.

2. Related work

2.1. Distributed and parallel evolutionary and swarm optimisation

The area of swarm optimisation is a growing field with innovative and multidisciplinary optimisation strategy focused in improving quality of solutions. Lin et al. [33] enhanced genetic learning particle swarm optimization enhances PSO by breeding better solutions to guide the motion of particles with diversity enhancement by ring topology. Liu et al. [34] modified particle swarm optimization using adaptive strategy to avoid the premature convergence, stochastic and mainstream learning strategies, an adaptive position updating strategy and terminal replacement mechanism for complex optimization problems. Roshanzamir et al. [35] presented hierarchical multi group particle swarm optimization with different task allocations inspired by holonic multi agent systems to improve their solutions.

In parallel computing, problem using separate parallel processors which may feature inter-process communication typically within a single machine [36]. Distributed computing on the other hand, considers several machines to break down a major task and therefore, distributed computing may also use parallel computing [37]. Distributed evolutionary algorithms and distributed swarms [38] typically refer to population distributed and dimension distributed models. Distributed evolutionary and swarm optimisation focuses in enhancing diversity of new populations and also to provide better computational efficiency especially in high high dimensional problems [39, 38].

Distributed and parallel optimisation has been steadily making progress. One of the earlier attempts was by Hereford [40] who presented distributed PSO suitable for a swarm consisting of a large number of small, mobile robots where each robot calculates its new position based on its present position and present measurement eliminating need for central agent and had limited inter-robot communication. Abadlia et al. [41] used island model concepts with PSO algorithm to improve its diversity and convergence, where the particles are distrusted into separate islands with exchange through a migration process. The results indicated that the island model provides improved efficiency of PSO performance. Decamps et al. presented parallel PSO strategies using Pareto dominance and decomposition based on multiple swarms for many-objective optimisation problems and investigated the impact of synchronous and asynchronous communication strategies for the decomposition-based approach. The results indicated that parallelization had a positive effect on the convergence and diversity of the optimization process. Erdeljan et al. presented a data model partitioning for parallelization of analytical power calculations using distributed PSO algorithms where results show that distributed PSO algorithm achieves significantly better results than the basic PSO algorithm.

2.2. Surrogate-assisted optimization

Surrogate-assisted optimisation has been initially motivated by computationally expensive engineering and design problems. Ong et al. [18] proposed parallel evolutionary optimisation with application to aerodynamic wing design where surrogate models used radial basis functions (RBF) networks. Zhou et al. [19] utilised global and local surrogate models for evolutionary optimization and improved performance. Lim et al. [44] accounted for uncertainty in estimation with a generalised method to unify diverse surrogate models. The search for an appropriate surrogate model is a major challenge given different forms of error or fitness landscape given by the actual model. Giunta et al. [45] compared surrogate models that used quadratic polynomial models with Gaussian process regression models (kriging) and found that the former gave more accurate estimation for the given optimisation problems. Jin et al. [46] compared several surrogate models where they reported radial basis functions as one of the best for scalability and robustness and kriging to be computationally expensive. There exists some comprehensive reviews about different categories of surrogate-assisted optimisation for different types of theoretical problems [17, 37] and applications in Earth science and water resource modelling [38].

Swarm optimisation is becoming prominent in surrogate assisted optimisation. Yu et al. [47] presented surrogate-assisted hierarchical particle swarm optimization with standard particle swarm optimization (PSO) and a social learning PSO for selected benchmark functions and demonstrated its competitiveness when compared with the state-of-the-art algorithms under a limited computational budget. Li et al. [48] presented a surrogate-assisted particle swarm optimization algorithm for computationally expensive problems where two criterion’s were applied in tandem to select candidates for exact evaluations. They include a performance-based criterion used to exploit the current global best and accelerate the convergence rate and a distance-based uncertainty-based criterion.
is used to enhance exploration that does not consider the fitness landscape of different problems. The results demonstrated better performance over several state-of-the-art algorithms for benchmark functions and propeller design problem was also used. Chen et. al [51] presented hierarchical surrogate-assisted differential evolution algorithm for high-dimensional expensive optimization problems with radial basis function network and benchmark functions were used and further application to oil reservoir production optimization problem provided promising results. Yi et. al [52] presented an on-line variable-fidelity surrogate-assisted harmony search algorithm with multi-level screening strategy that outperformed related methods and showed promising performance for expensive engineering design optimization that featured design for a long cylindrical gas-pressure vessel.

Further work using swarm optimisation is part of latest research. Li et. al [53] presented ensemble of surrogates assisted particle swarm optimization of medium scale expensive problems which used multiple trial positions for each particle and selected the promising positions by using the superiority and uncertainty of the ensemble simultaneously. In order to feature faster convergence and to avoid wrong global attraction of models, the optima of two surrogates that featured polynomial regression and radial basis function models were evaluated in the convergence state of particles. Liao et. al [54] presented multi-surrogate multi-tasking optimization of expensive problems to accelerate the convergence by regarding the two surrogates as two related tasks. Therefore, two optimal solutions found by the multi-tasking algorithm was evaluated using the real expensive objective function, and both the global and local models are updated until the allowed computational budget is exhausted. The results indicated competitive performance with faster convergence that scales well with the increase in problem dimension for solving computationally expensive single-objective optimization problems. Dong et. al [55] presented surrogate-assisted grey wolf optimization for high-dimensional and computationally expensive black-box problems that featured RBF-assisted meta-heuristic exploration. The RBF featured knowledge mining that includes a global search carried out using the grey wolf optimization and a local search strategy combining global and multi-start local exploration. The method obtained superior computation efficiency and robustness demonstrated by comparison tests with benchmark functions. Chen et. al [51] presented efficient hierarchical surrogate-assisted differential evolution for high-dimensional expensive optimization using global and local surrogate model featuring RBF network with an application to an oil reservoir production optimization problem. The results show that the method was effective for most benchmark functions and gave promising performance for reservoir production optimization problem.

Some of the prominent examples for surrogate assisted approaches in the Earth sciences include modeling water resources [48, 56], computational oceanography [57], atmospheric general circulation models [58], carbon-dioxide storage and oil recovery [59], and debris flow models [60].

2.3. Landscape evolution models and Bayeslands

Landscape evolution models (LEMs) use different climate and geophysical aspects such as tectonics or climate variability [61, 62, 63, 64, 65] and combine empirical data and conceptual methods into a set of mathematical equations that form the basis for driving model simulation. Bayeslands (basin and landscape dynamics) [63, 66] is a LEM that simulates landscape evolution and sediment transport/deposition [67, 68] with an initial topography exposed to climate and geological factors over time with given conditions (parameters) such as the precipitation rate and rock erodibility coefficient. The major challenge is in estimating the climate and geological parameters and those that are linked with the initial topography since they can range millions of years in geological timescale depending on the problem. A way is to develop an optimisation framework that utilize limited data. Since gradient information is not available, Badlands can be seen as a black-box optimisation model where the unknown parameters need to be found via optimisation or Bayesian inference. So far, the problem has been approached with Bayesian inference that employs MCMC sampling for estimation of these parameters in a framework known as Bayeslands [69].

The Bayeslands framework had limitations due to computational complexity of Badlands model, hence it was extended using parallel tempering MCMC [70] that featured parallel computing to enhance computational efficiency and sampling. Although we used parallel computing with small-scale synthetic Badlands model, the procedure remained computationally challenging since thousands of samples were drawn and evaluated. Running a single large scale real-world Badlands model can take several minutes to hours, and even several days depending on the area covered by the landscape evolution considered and the span of geological time considered in terms of millions of years. Therefore, parallel tempering Bayeslands was further enhanced through surrogate-assisted estimation. We used developed surrogate-assisted parallel tempering has for landscape evolution models where a global-local surrogate framework utilised surrogate training in the main process that managed MCMC replicas running in parallel [52]. We obtained promising results where prediction performance was maintained while lowering computational time using surrogates for synthetic examples that also featured landscape evolution of Tasmania over a million years.

3. Surrogate-assisted distributed swarm optimisation

3.1. Particle Swarm Optimisation

Particle swarm optimisation (PSO) is a population based metaheuristic that improves the population over iterations with a given measure of accuracy known as fitness [71]. The population of candidate solution in PSO is known as swarm while the candidate solutions are known as particles that get updated according to the particle’s position and velocity. In the swarm, each particle’s movement is typically influenced by its local best known position, but also guided toward the best known positions that get updated when better positions are discovered
by other particles. Equations [1] and [2] show the velocity and position update of the particle in a swarm, respectively.

\[ \mathbf{v}_{t+1} = \alpha \mathbf{v}_t + c_1 \gamma_1 (\mathbf{x}_{pbest} - \mathbf{x}_t) + c_2 \gamma_2 (\mathbf{x}_{gbest} - \mathbf{x}_t) \]  

\[ \mathbf{x}_{t+1} = \mathbf{x}_t + \mathbf{v}_{t+1} \]  

where \( \mathbf{v}_t \), \( \mathbf{x}_t \) represent the velocity and position of a particle at time step \( t \), respectively. \( c_1 \) and \( c_2 \) are the user-defined cognitive and social acceleration coefficients, respectively. \( \gamma_1 \) and \( \gamma_2 \) are random numbers drawn from uniform \( U[0, 1] \) distribution, and \( \alpha \) is the user-defined inertia weight. There are several variants in the way the particles get updated which have their own strengths and limitations for different types of problems [71][72][73][74][75].

### 3.2. Surrogate assisted Distributed framework

We use a canonical particle update method [71] where the swarms are executed in parallel computing framework as a separate process.

#### 3.2.1. Inter Process Communication

In our distributed swarm framework that used parallel computing, we exchange selected swarm particles after certain number of generations with inter-process communication. During the exchange, we replace 20 percent of the weaker particles by stronger ones from other swarm. This provides another mode of search space exploration and exploitation to our optimization problem. Afterwards, the process continues where local swarms create particles with new position and velocity as shown in Figure [1]. Hence, we feature distributed swarms and parallel processing for better diversity and computational complexity. We execute distinct parallel process for respective swarms with central processing units (CPUs) if enough are present or be shared. Each processing core features the optimisation function which is synthetic benchmark problem made to be computationally expensive or application problem with data and swarms which communicates with the master or manager process.

#### 3.2.2. Use of Surrogate Model

Suppose that the true function or model is represented as \( F = g(x) \) where \( g() \) is the function and \( x \) is a solution or particle from a given swarm. Our surrogate model outputs pseudo-fitness \( \hat{F} = \hat{g}(x) \) that would give an approximation of the true function via \( F = \hat{F} + e \), where \( e \) represents the difference between the surrogate and true function. The surrogate model gives an estimate using the pseudo-fitness for replacing true-function when required by the framework. \( S_{prob} \) is an important hyperparameter which controls use of surrogate in the prediction, neither want it to be too high in case we are not very confident about our surrogate model as then the optimization will become random nor we want it to be too low as then the process will become time consuming. Hence we need to tune this parameter. Surrogate model is trained accumulating the data from all the swarms, i.e. the evaluated input \( \mathbf{x}_s \) and associated true-fitness \( F_{s,i} \) pairs; where \( s \) represents the particle and \( i \) represents the swarm. To take benefit from the surrogate in the optimization process its very crucial to manage the surrogate training and surrogate use. We cannot use surrogate from the very start of the optimization as its predictions will be random, neither we can wait too long as the purpose of computational efficiency will be defeated then. Hence to manage the surrogate training and its use, an important hyperparameter \( \psi \) is used, \( \psi \) is the surrogate interval measured in terms of number of generations, it is the interval after which all the collected data is used to train the model, this updated model is used as the surrogate till the next interval is reached. The collected input features (\( \mathbf{Φ} \)) combined with the true fitness \( \lambda \) create \( \theta \) for the surrogate model.

\[ \mathbf{Φ} = ([x_{1s}, \ldots, x_{1s+\psi}], \ldots, [x_{Ms}, \ldots, x_{Ms+\psi}]) \]

\[ \lambda = ([F_{1s}, \ldots, F_{1s+\psi}], \ldots, [F_{Ms}, \ldots, F_{Ms+\psi}]) \]

\[ \Theta = [\mathbf{Φ}, \lambda] \]  

where \( x_{is} \) represents the given particle from the swarm, \( s \), \( F_{is} \) is the output from the true-fitness, and \( M \) is the number of swarms. Therefore, the surrogate training dataset (\( \Theta = [\mathbf{Φ}, \lambda] \)) is made up of input features (\( \mathbf{Φ} \)) and response (\( \lambda \)) for the particles that get collected in each surrogate interval \((s + \psi)\). Our pseudo-fitness is given by \( \hat{y} = \hat{F}(\mathbf{θ}) \).

#### 3.2.3. Proposed Framework

In Algorithm [1] we present further details about the methodology that features surrogate assisted optimisation using distributed swarms.

We implement the algorithm using distributed computation over CPU cores, as shown in Algorithm [1] the manager process is in blue where inter-process communication among swarms takes place which exchange parameters at regular intervals (given by \( \psi \)) and surrogate model is trained at regular intervals (\( \psi \)). The parallel swarms have been highlighted in pink in Algorithm [1] Stage 0 features the initialization of particles in the swarm. We begin optimisation process by initialising all the respective swarms (Stage 0.1) in the ensemble with random real numbers in a range depending on the optimisation function or model. Once the swarms are initialised, we begin the evolution (optimisation) by first evaluating the particles in the swarms using the fitness (objective) function. We note that we update the best particle and best fitness for each of the respective swarms in the ensemble afterwards. Once these basic operations are done, we begin the evolution process where we create a new set of swarms for the next generation by velocity and position update (Stage 1.1).

The crux of the method is when we consider whether to evaluate the fitness function (true fitness) or to use the surrogate model of the fitness function (pseudo-fitness) when computing fitness values. Stage 1.2 shows how to update the fitness using either surrogate or true fitness of particle depending on the interval and \( S_{prob} \), initially till the very first surrogate interval is not reached all evaluations will be from true function. In Stage 1.3, we calculate the moving average of past three fitness values for a particular particle by \( F_{past} = mean(F_{s-1}, F_{s-2}, F_{s-3}) \) to combine with surrogate model prediction (Stage 1.4). In Stage
1.5 and 1.6, we calculate actual fitness and save the values for future surrogate training. Our swarm particle update depends on \(x_{\text{pbest}}^i\) and \(x_{\text{gbest}}^i\), it may happen due to poor surrogate performance some bad particles get high fitness score. In order to avoid this issue, we ensure that \(x_{\text{pbest}}^i\) and \(x_{\text{gbest}}^i\) are from true fitness evaluation. In Stage 2.0, given a regular interval \((\phi)\), we prepare exchange of selected particles with neighboring swarms where we replace a given percentage of weak particles (given by fitness values) to ensure elitism.

We note that before we consider the use of pseudo-fitness, we need to train the surrogate model with same training data which is created from the true fitness. Hence we need to collect the training data for the surrogate model from all the swarms in the ensemble. Hence, in Stage 3.0, the algorithm uses surrogate training data collected from Stage 1.6 \((\Theta)\) as shown in Equation 3. In Stage 4, the algorithm trains the surrogate model in the manager process with data from Stage 3. The knowledge from trained surrogate model is then used in the fitness estimation as shown in Stage 1.4.

Stage 5.0 executed the termination condition where the algorithm signals the manager process to decrement number of swarms alive to terminate the swarm process, when maximum number of evaluations has been reached \((T_{\text{max}})\). We use neural network based surrogate model with Adam optimisation [65]. In order to validate the performance of the algorithm, we measure the quality of the surrogate estimate using the root mean squared error (RMSE):

\[
\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (F_i - \hat{F}_i)^2}
\]

where \(F_i\) and \(\hat{F}_i\) are the true and pseudo-fitness values, respectively. \(N\) denotes the number of times the surrogate model is used for estimation.

Figure 1 provides visual description of the proposed algorithm. Multiple swarms consisting of updating population are managed using the manager process which keeps control of particle exchange and surrogate model update. All the details are marked in the figure.

4. Application: Landscape evolution models

Other than optimizing mathematical functions many a time we are required to evaluate a score using some simulation or other computationally expensive process, an example of which are Landscape evolution models (LEMs). They typically require an initial topography that is evolved over given time with given geological and climate conditions such as rock erodibility and precipitation [63]. LEMs are used to model and understand the landscape and basin evolution back in time over millions of years showing surface process such as formation of river systems and erosion/deposition where there is movement of sediments from source (mountains) to sink (basins) [29]. LEMs help geologists and paleoclimate scientists understand the evolution of the planet and climate history over millions to billions of years; however, there are major challenges when it comes to data. LEMs generally require data regarding paleoclimate processes which is unavailable and hence we need to estimate them with methods such as Bayesian inference [76, 77]. There has not been any work in the literature where optimisation methods can be used to estimate the unknown parameters for LEMs, which is the focus of this study. We note that typically, LEMs are computationally very expensive which is dependent on the resolution of the study area (points/kilometer) and how how the evolution goes back in time (millions of years). Hence, large scale study areas can take from hours to days to run a single model even while using parallel computing [63]. There is typically no gradient information in case of Badlands LEM used for this study, and hence estimating the parameters is a challenge.

In order to demonstrate the optimisation procedure, we select problems where synthetic initial topography is created using present day topography or synthetically generated and used in our previous work [76, 77]. The selected LEM features a continental margin (CM) problem that is selected taking into account computational time of a single model run as it takes less than three seconds on a single central processing unit (CPU). The CM problem initial topography is selected from present-day South Island of New Zealand as shown in Figure 2 which covers 136 by 123 kilometers. We provide a visualization of the initial and final topographies along with erosion/deposition map for CM problem, in Figure 3. The CM features six free parameters (Table 1). Notable feature in all three problems is that they model both the elevation and erosion/deposition topography. We use the initial topography (Figure 5) and true values in Table 1 and run the Badlands LEM simulating 1 million years to synthetically generate ground-truth topography. We then create a fitness function with the ground-truth topography and set experiments so that the proposed optimisation methods can get back the true values. The details about the fitness function is given in the following section.

4.1. Fitness function

The Badlands LEM produces a simulation of successive time-dependent topographies; however, only the final topography \(D_T\) is used for topography fitness since no successive ground-truth data is available. The sedimentation (erosion/deposition) data is typically used to ground-truth the time-
**Result:** Fitness Score

* Set the number of swarms \( (M) \) in ensemble as alive; alive = \( M \)
* Define the swarm population size \( (pop\_size) \), limits of parameters \( (maxx, minx) \), number of swarm processes \( (M) \), surrogate interval \( (\phi) \), swap-interval \( (\psi) \), and maximum swarm evaluations \( (T_{\text{max}}) \).

\[
\text{while} \ (\text{alive} \neq 0) \text{ do}
\]
  Prepare manager process to execute swarms in parallel cores

\[
\text{for each } m \text{ until } M \text{ do}
\]

\[
\text{evals} = 0
\]

**Stage 0:** Initialization of parameters

\[
\text{for each } i \text{ until } pop\_size \text{ do}
\]

1. Initialize the position and velocity of particle \( x_i, v_i \) respectively given the bound.
2. Initialize \( x_i^{\text{pbest}} = x_i, \delta_i = F(x_i), \delta_i^{\text{best}} = \delta_i \).

end

Compute \( \delta_i, x_i^{\text{gbest}} \) among the swarm particles with best fitness and its corresponding parameter.

\[
\text{while} \ (\text{evals} < T_{\text{max}}) \text{ do}
\]

**Stage 1.0:** PSO

\[
\text{for each } v \text{ until } \psi \text{ do}
\]

\[
\text{for each } k \text{ until } \phi \text{ do}
\]

\[
\text{for each } i \text{ until } pop\_size \text{ do}
\]

1. Update \( x_i, v_i \) via PSO update rule as in equation 1 and 2

2. Check the parameters bounds using \( minx \) and \( maxx \).

3. Estimate \( F_i \):

   a. Draw \( \kappa \) from a Uniform distribution \([0,1]\)
   b. if \( \kappa < S_{\text{prob}} \) and \( \text{evals} > \psi \) then
      \[ F_{\text{pseudo}} = F(x_i) \]
   c. else
      \[ F_{\text{past}} = \text{mean of fitness values of particle } x_i \text{ for last three generations} \]

\[
\text{else}
\]

\[
\delta_i^{\text{best}} = \delta_i, x_i^{\text{gbest}} \leftarrow x_i
\]

\[
\delta_i \leftarrow \delta_i^{\text{best}}, x_i^{\text{pbest}} \leftarrow \delta_i
\]

end

4. Increment \( \text{evals} = \text{evals} + \text{pop}\_size \)

end

**Stage 2.0:** Neighbouring swarm exchange:

1. Use a swapping probability \( \beta \) and draw \( b \) from a Uniform distribution \([0,1]\)
2. if \( b \leq \beta \) then

   \[
   2.1 \text{ Signal()} \text{ manager process}
   \]

   \[
   2.2 \text{ Exchange some parameters with neighbouring swarms, } \theta_m \leftrightarrow \theta_{m+1}
   \]

end

**Stage 3.0:** Collect data \( \Theta_m \) which features history of parameters \( \Phi(x) \) and fitness response \( \lambda (F_i) \) using data collected from Stage 1.6

**Stage 4.0:** Train global surrogate model

\[
\text{for each island do}
\]

1. Get swarm training data \( \Theta_m \) from Stage 3.0

end

2. Train surrogate model, \( \Upsilon = [\Theta_1, \Theta_2, ..., \Theta_M] \).

3. Store surrogate model, \( \Psi \)

end

**Stage 5.0:** Signal() the manager process

1. Decrement the number of swarms alive

end

**Stage 6:** Combine predictions for particle in the swarm with best fitness from different islands in the ensemble.

**Algorithm 1:** Surrogate assisted swarm optimization for computationally expensive models.
Figure 1: Surrogate-assisted distributed swarm optimisation features surrogates to estimate the fitness of expensive models or functions.

| Issue         | Rainfall (m/a) | Erod. | n-value | m-value | c-marine | c-surface | Uplift (mm/a) |
|---------------|----------------|-------|---------|---------|----------|-----------|---------------|
| True-values   | 1.5            | 5.0e-06 | 1.0     | 0.5     | 0.5      | 0.8       | -             |
| Limits        | [0, 3.0]       | [3.0e-06, 7.0e-06] | [0, 2.0] | [0, 2.0] | [0.3, 0.7] | [0.6, 1.0] | -             |

Table 1: True values and limits of parameters.
dependent evolution of surface process models that include sediment transportation and deposition [63, 69].

We adapt the fitness function from the likelihood function used in our previous work that used Bayesian inference via Markov Chain Monte-Carlo sampling algorithm for parameter estimation in Badlands model [76]. The initial topography is given as $D_0$ with $D_0 = (D_{0,1}, \ldots, D_{0,n})$, where $s_i$ corresponds to the location which is given by the latitude $u_i$ and longitude $v_i$ (eg. Figure 2). Hence, our topography fitness function $F_{\text{topo}}$ for the topography at final time $t = T$ is given by

$$F_{\text{topo}}(\theta) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (D_{s_i, T} - f_{s_i, T}(\theta))^2} \quad (4)$$

where $N$ is the number of observations.

The sediment erosion/deposition values at time $(z_t)$ are simulated (predicted) by the Badlands model when given set of parameters, $\theta$. The sediment fitness $F_{\text{sed}}(\theta)$ is given below

$$F_{\text{sed}}(\theta) = \sqrt{\frac{1}{(T + J) \sum_{t=1}^{T} \sum_{j=1}^{J} (z_{s,j,t} - g_{s,j,t}(\theta))^2}} \quad (5)$$

5. Experiments and Results

In this section, we present analysis of the proposed methodology first on synthetic benchmark functions then on Badlands(LEM). The experiments consider a wide range of performance measures which includes optimization performance in terms of fitness score, computational time saved by the surrogate model, accuracy of the surrogate model.

5.1. Experiment design

We provide the experimental design and parameter setting for our experiment as follows. We implement distributed swarm
optimization using parallel computing and inter-process communication where the swarms can have separate process and exchange solutions (particles) with Python multi-processing library.

The synthetic benchmark optimisation functions are given in Equation 6 (Spherical), Equation 7 (Ackley), Equation 8 (Rastrigin), and Equation 9 (Rosenbrock). Note that these functions are chosen due to different level of difficulty in optimisation and difference in nature of their error or fitness landscape. Spherical function is considered to be an relatively easier optimisation problem since it does not have interacting variables. Ackley and Rastrigin are known to be many local minima functions, while Rosenbrock is known as the valley shaped function.

\[ f(x) = f(x_1, x_2, \ldots, x_n) = \sum_{i=1}^{n} x_i^2 \]  

\[ f(x) = \sum_{i=1}^{n} \left[ b(x_i) - x_i^2 \right]^2 + (a - x_i)^2 \]  

\[ f(x) = -a + \exp(-b \left( \frac{1}{n} \sum_{i=1}^{n} x_i^2 \right) - \exp(\frac{1}{n} \sum_{i=1}^{n} \cos(cx_i))) + a + \exp(1) \]  

\[ f(x) = 10n + \sum_{i=1}^{n} (x_i^2 - 10\cos(2\pi x_i)) \]

We use (M=8) swarms which run as parallel processes (swarms) that inter-communicate with each other at regular interval where we exchange a subset of particles (best 20% from the population) with the neighbouring island (worst 20% of the population). We use the population size of 20 particles per swarm, the inertia weight of 0.729 with social and cognitive coefficients (c1=1.4 and c2=1.4). We determined these values for parameters in the trial experiments by taking into account the performance on different problems with a fixed number of evaluations. We used minimum and maximum bound on the parameters as described in the table, respectively. We ran experiments for 30 dimensions (30D) and 50D versions of the respective benchmark problems where the total number of function evaluations were set to 100 000 and 200 000, respectively. In the case of Badlands model, we used 10 000 function evaluations for our problem instance, CM.

We used the PyTorch machine learning library for implementing the surrogate model that uses a neural network model with Adam learning. The surrogate neural network model architecture is given in Table 2 where the input dimensions are defined by the dimension of the problem used i.e. 30D or 50D for two different instances of the synthetic benchmark problems. In a similar way, we extend our approach for optimization in Badlands model where we have CM problems, featuring 6D search space. The first and second hidden layers of the of the neural network based surrogate model is shown in Table 2. We note that the output layer in the model for all problems contains only one unit which provides the estimated fitness score.

| Problem | Hidden(h1) | Hidden(h2) |
|---------|------------|------------|
| Rosenbrock 30D | 30 | 15 |
| Rastrigin 30D | 30 | 15 |
| Ackley 30D | 30 | 15 |
| Spherical 30D | 30 | 15 |
| Rosenbrock 50D | 50 | 25 |
| Rastrigin 50D | 50 | 25 |
| Ackley 50D | 50 | 25 |
| Spherical 50D | 50 | 25 |
| Badlands | 20 | 10 |

5.2. Results for synthetic benchmark functions

We first present the results (fitness score) for different problems using canonical serial PSO, distributed PSO (D-PSO) and surrogate-assisted distributed swarm optimisation (SD-PSO) as shown in Table 3. We use a fixed surrogate probability (s_prob = 0.5) and present results featuring mean, standard deviation (std), best and worst performance for over 30 independent experimental runs with different random initialisation in swarms as shown in Table 3. Note the lower fitness scores provides better performance.

We find significant reduction in elapsed time for all the problems in Table 3. We note that a 0.05 seconds time delay was added to the respective problems to make them slightly computationally expensive to depict real-world problems that could take more time. When we consider serial PSO with D-PSO and SD-PSO in the terms of optimisation performance given by the fitness score, we find that D-PSO improves the PSO significantly for 30D and 50D cases of Rosenbrock, Spherical and Rastrigin problems. We also see improvement in Ackley problem, but its not as large as in previous problems. We find the variation in the results given by the standard deviation is lowered highly with D-PSO which shows it is more robust to initialization and has the ability to provide more definitive solution.

Moreover, we compare the results of the SD-PSO with D-PSO and observe that overall we get similar or better results with SD-PSO, with reduction of computation time due to the use of surrogates. Despite the use of surrogate-based fitness estimation, we observe that the fitness-score has not greatly depreciated. It is interesting to note in Ackley 30 and 50D case, addition of surrogates is improved the fitness score. We see a 30% reduction in computational time, it is expected that this reduction will increase if we had more time delay (rather than 0.05 seconds) which will will see in experiments to follow.

The RMSE of prediction of fitness by surrogate model is shown in Table 4. We notice large RMSE values for Rosenbrock problem when compared to the rest. In surrogate prediction accuracy (RMSE) given in Figure 5, we observe a constant reduction in RMSE with intervals (along x-axis) in Ackley (30D and 50D), and Spherical (30D) model functions. In other
problems, the RMSE is lower towards the end, but trend is not that smooth. We note that in Rosenbrock model, there exists an interval where our surrogate performs poorly causing major decrease in accuracy.

Figure 3 and 7 provide a visual description surrogates prediction quality in the evolution process. We show the bar plots for mean values with 95% confidence interval (shown by error bars) of actual fitness and pseudo-fitness at regular intervals for different benchmark problems. We notice that Rastrigin and Ackley problems have a better surrogate prediction with better confidence intervals when compared to the Spherical problem. Finally, we evaluate the effect of surrogate probability for Rosenbrock and Rastrigin 3D problems. Figure 4 (Panel a) provides graphical analysis of how our fitness score change with varying surrogate probabilities and computational time is shown as well (Panel b). We observed that the computational time decreases linearly with surrogate probability. On the other hand, the fitness score degrades with surrogate probability, but with an elbow shaped curve and a trade off can exist between time and optimization performance, which is at surrogate probability of 0.5.

5.3. Results for the Badlands model

Finally, we present results for the case of the Badlands CM problem which is a 6D problem. The results for CM problem highlighting our methods (PSO, D-PSO and S-DPSO) when compared to previous approaches (PT-Bayeslands and SAPT-Bayeslands) are shown in Table 5. The results show the computational time and prediction performance of the Badlands model in terms of elevation and erosion/deposition RMSE (using Equation 4 and 5, respectively) given the optimised parameters. The results show the mean and standard deviation from 30 experimental runs from independent initial positions. We see major reduction in computational time using DPSO when compared to PSO and find consistent performance in terms of elevation and erosion RMSE. The experiments used surrogate model at an interval of 10 generations with probability of 0.5. We observe that the S-DPSO further improved the performance in terms of computational time and efficient as shown. The RMSE of the estimation of fitness function by the surrogate model when compared to the actual Badlands model is shown in Table 4. We note that the RMSE here cannot be compared to the synthetic fitness functions (eg. Rosenbrock) since the fitness function is completely different. In synthetic fitness functions, there is no data whereas in Badlands LEM, we use Badlands prediction and ground-truth topography data to compute the fitness. Figure 7 (Panel c) shows surrogate training accuracy (RMSE) for different surrogate intervals where we observe a constant improvement of performance by surrogate model over time (surrogate intervals). This implies that the surrogate model is improving as it gathers more data over time.

In Figure 8 we show the change in CM topology over selected time-slices simulated by Badlands according to the parameters optimized by S-DPSO. The elevation RMSE in 6 considers the difference between ground-truth topography given in Figure 5. We notice that visually the final topography (present day) in Figure 5 (Panel f) resembles Figure 3 (Panel b). Furthermore, we show in Figure 6 a cross-section (Panel a) for Badlands predicted elevation vs the ground-truth elevation for final or present day topography. We also show the bar-plot (Panel b) of predicted vs ground-truth sediment erosion/deposition at 10 selected locations taken from Figure 5 (Panel c). The cross-section and bar-plots show that the Badlands prediction well resembled the ground-truth data, respectively. We observe that the cross-section (Panel a) uncertainty is higher for certain locations as highlighted. The high uncertainty is in area of high slope below seal-level which is reasonable given effect of sediment flow due to precipitation.

6. Discussion

Overall, the results show that distributed swarm optimisation can be improved in performance such as decrease computation time while retaining optimisation accuracy (fitness) using our proposed surrogate-assisted distributed swarm optimisation. We also found that the use of surrogates may even boost performance in terms of optimisation accuracy as in case of Spherical, and Ackley functions (Table 3), and Badlands landscape evolution model problem (Table 5). This might be due to smooth approximation of the problem by our surrogate model which prevented the optimization process in trapping in local minima. We highlight that the Badlands model does not provide gradient information regarding the parameters and hence only gradient free optimisation or inference methods can be used. In previous work, we used MCMC methods (PT-Bayeslands and SAPT-Bayeslands [69,70]) where the search was done via random-walk proposal distribution with MCMC replicas running in parallel. Our results show that the use of meta-heuristic search operators from particle swarm optimisation provides better search features. The results motivates the use the proposed methodology for expansive optimisation models, which can feature other geoscientic models. Further use of surrogate in larger instances of the Badlands landscape evolution model can provide significant reduction in computational time.

A major contribution of the methodology has been in the implementation using parallel computing, which takes into account inter-process communication when exchanging particles (solutions) during the optimisation process. In our proposed framework, the surrogate training was implemented in the manager process and the trained parameters were transferred to the parallel swarm processes where local surrogate model was used to estimate the fitness of the particle when required (Figure 1). This implementation had to seamlessly update the local surrogate model at regular intervals set by the user. We note that although less than eight parallel swarm processes were used, in large scale problems, the same implementation can be extended and amended. We note that in case when the number of parameters in the actual model used for optimisation significantly increases, different ways of training the surrogate model can be explored.

Another major contribution from the optimisation process for the case of landscape evolution model is the inference of the
Figure 4: The figure shows effect of surrogate probability on fitness score and computational time.

Table 3: Optimization Results on benchmark functions

| Problem    | Method      | Fitness Score | Elapsed Time |
|------------|-------------|---------------|--------------|
|            |             | [mean std best worst] (minutes) |              |
| Rosenbrock 30D | PSO         | 183.95 109.94 60.88 455.01 | 84.39        |
|             | D-PSO       | 108.78 38.0 55.0 178.0 | 11.22        |
|             | SD-PSO (0.5) | 149.7 50.91 67.92 270.18 | 7.113        |
| Rosenbrock 50D | PSO         | 1285.41 559.54 432.89 2519.02 | 84.37        |
|             | D-PSO       | 1269.03 390.0 78.0 2084.0 | 11.24        |
|             | SD-PSO (0.5) | 2449.32 1093.8 685.48 5298.79 | 7.114        |
| Spherical 30D | PSO         | 9.06 9.22 1.43 37.85 | 84.35        |
|             | D-PSO       | 4.79 3.0 1.0 12.0 | 11.31        |
|             | SD-PSO      | 1.82 0.74 0.9 3.33 | 7.112        |
| Spherical 50D | PSO         | 252.96 102.69 67.75 426.74 | 84.38        |
|             | D-PSO       | 175.2 45.0 118.0 256.0 | 11.23        |
|             | SD-PSO (0.5) | 111.85 48.36 34.05 239.828 | 7.113        |
| Rastrigin 30D | PSO         | 72.33 19.72 27.05 112.21 | 84.38        |
|             | D-PSO       | 62.61 12.0 41.0 90.0 | 11.20        |
|             | SD-PSO (0.5) | 77.23 12.57 52.96 107.26 | 7.113        |
| Rastrigin 50D | PSO         | 188.34 33.83 130.96 257.53 | 84.39        |
|             | D-PSO       | 180.7 24.0 122.0 215.0 | 11.1         |
|             | SD-PSO (0.5) | 243.73 25.1 192.2 307.82 | 7.114        |
| Ackley 30D  | PSO         | 2.32 0.39 1.66 3.03 | 84.37        |
|             | D-PSO       | 1.83 0.0 1.0 2.0 | 11.21        |
|             | SD-PSO (0.5) | 1.66 0.33 0.99 2.24 | 7.112        |
| Ackley 50D  | PSO         | 3.8 0.38 3.24 4.58 | 84.38        |
|             | D-PSO       | 3.42 0.0 3.0 4.0 | 11.21        |
|             | SD-PSO (0.5) | 3.34 0.23 2.76 3.73 | 7.113        |
Figure 5: RMSE of surrogate training during different surrogate intervals.
Figure 6: Surrogate fitness versus actual fitness score over number of fitness evaluations (surrogate evaluations) for different problems.
Figure 7: Surrogate fitness versus actual fitness score over number of fitness evaluations (surrogate evaluations) for different problems.
Figure 8: This is how topology evolves according to our badlands model optimized using S-DPSO. Note that the distance over x-axis and y-axis is given in kilometers (km) and the elevation is given in meters (m).
parameters, such as precipitation values in the Badlands model. Through optimisation, we can estimate what precipitation values gave rise to the evolution of landscape which resulted in present day landscape. The landscape evolution model hence provides a temporal topography map of the geological history of the region under study, and eventually the planet given data availability which is a major challenge in geoscience. These topographical maps, along with the optimised values for geological and climate parameters (such as precipitation and erodibility) can be very useful to geologies and climate scientists who study ancient climates.

7. Conclusions and Future Work

We presented a surrogate framework that features parallel swarm optimisation processes and seamlessly integrates surrogate training from the manager process to enable surrogate fitness estimation. Our results indicate that the proposed surrogate-assisted optimisation method significantly reduces the computational time, while retaining solution accuracy. In certain cases, it also helps in improving the solution accuracy by escaping from local minimum via the surrogates. Although we used particle swarm optimisation as the designated algorithm, other optimisation algorithms, such as genetic algorithms, evolution strategies and differential evolution can also be used.

In future work, the parallel optimisation process could be improved by a combination of different optimisation algorithms which can provide different capabilities in terms of exploration and exploitation of the search space. The proposed framework can also incorporate other benchmark function models, particularly those that feature constraints and also be applied to discrete parameter optimisation problems which are expensive computationally.

### Software and Data

We provide an open-source implementation of the proposed algorithm in Python along with data and sample results[^1]

### Acknowledgement

The authors would like to thank Ratneel Deo for support during the initial phase of this research project.

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[^1]: Surrogate-assisted distributed evolutionary algo: https://github.com/sydney-machine-learning/surrogate-assisted-distributed-evo-alg
Figure 9: Prediction cross-section (Panel a) and sediment erosion/deposition (Panel b) with uncertainty given as 95% confidence interval from 30 experimental runs.

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