**Abstract**

This document addresses the need for increased efficiency in optimizing computationally expensive black-box problems and proposes a surrogate model-based differential evolution algorithm for multi-objective optimization. The surrogate models applied here are the Gaussian Process (GP) models. The algorithm is aimed at finding nondominated solutions to computationally expensive problems using approximation within certain confidence limits by preparing & updating GP models of objectives using reduced number of objective evaluations. The NSDE-GP algorithm has been tested on multiple benchmarking problems and expensive black-box problems. The performance of the algorithm has been tested against two evolutionary meta-heuristics – the Real Non-Dominated Sorting Genetic Algorithm-III (RNSGA-III) (Deb & Jain, 2014) and the Non-Dominated Sorting Differential Evolution Algorithm (NSDE), and a surrogate model-based algorithm – the Surrogate Optimization of Computationally Expensive Multi-Objective Problems (SOCEMO).

<Mention discussion of results in short>

1. **Introduction**

Black Box problems – situations where only the inputs and outputs can be visualized but the internals are not comprehensible, are encountered in a plethora of domains in engineering and beyond. Selecting the right inputs to get the best desired outputs is tricky for such problems, especially when multiple objectives are to be achieved. Many computationally expensive & complex systems are usually perceived as black boxes - such as complex electrical circuits, highly composite functions, cryptographic models, etc. In case of optimization of multiple objectives, we do not get a single solution, but a family of non-dominated solutions known as the Pareto Optimal set. The user can pick one of these non-dominated points based on his/her priority.

Optimization Algorithms have been used since long, for optimizing industrial processes, reducing energy consumption, in finance economics (such as game-theory, etc.) and many other domains. Evolutionary Algorithms (EAs) are one of the most popular and effective methods to solve such multi-objective problems. These algorithms are actually metaheuristics inspired from natural phenomena of evolution and search. A multitude of optimization algorithms inspired by physical and social phenomenon have been developed in the last few decades. While most of these algorithms claim convergence in optimization problems, they mostly lack a promise of being efficient for most commonly encountered optimization problems in real-life. These algorithms usually depend on converging by performing a large number of problem evaluations, which create high CPU costs.

However, by approximating the black box formulation as a surrogate model using lower number of data points (and thus less evaluations), we can find optimal solution in lesser time. Over the decades, surrogate models have been largely utilized in simulation, prediction, automation applications. They also help to improve tractability of analytical procedures or libraries. The possibilities of application of surrogate models are endless, and with increasing collection of process/user data from a plethora of sources, these modelling techniques are proving to be more & more relevant & effective.

Among a variety of available surrogate models for optimization such as Polynomial Response (PR) models, ANNs, kriging, superiority cannot be established in most cases. However, one ca ………...

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For probabilistic models, the efficiency of a set of approximated solutions can be evaluated by defining a confidence interval of the approximation. This confidence interval can then be used to further define dominance conditions for the approximations, so that expensive evaluations are performed only when required confidence is not achieved.

1. Related Work

Optimization using “Surrogate Model(s)”, throughout the literature, aims at creating a model of the actual problem, thus reducing the number of actual objective evaluations. While in the single-objective case, these models predict one optimal value, one gets a nondominated set in case of multi-objectives.

For single objective optimization, surrogate models have proved to be effective over non-surrogate model meta-heuristics on benchmark problems. Techniques such as Kriging and PRS have been superior to the ones not using surrogates. [Jin, Olhofer, &Sendhoff,2001; Zhou Ong, Nair, Keane & Lum,2007]. The most widely used surrogate models are the Kriging [(Stein,1999], Polynomial Response Surface [], Radial Basis Functions (RBF) [], and the Gaussian Process Models[].

Combination techniques of surrogate models and metaheuristics have been known since the last decade. Ratle[] used a simple GA-Kriging combination strategy, and Liang et al. [] coupled EA with a quadratic response surface model. In [Zhou et. Al. 2007], the authors used a Data-parallel Gaussian Process (DPGP) technique to select better individuals in an EA, and subsequently used a Radial Basis Function (RBF) model to enhance local search. The concept of *evolution control* was introduced by [Jin, 2003], and its fixed variant was later used by Deb & Nain. 2007 in an Artificial Neural Network (ANN)-based approach. In evolution control, the model quality is estimated to alter the balance between dependency on approximate model and actual fitness function. In fixed evolution control, this balance is pre-defined, while in *adaptive* control, a dynamic method to adjust the frequency of control is employed using repeated assessment of model quality.

For Kriging model, improvement of model accuracy can be achieved through optimization of parameters such as Expected Improvement (EI) [Jones et al.], the Expected Hypervolume Improvement (EHVI)[ Emmerich et al.] and Estimate (EST) [Li et al]. Comparison of the three parameters by [Luo et. Al.] on a variety of multi-objective benchmark problems in multiple dimensions suggested that the performance was in the decreasing order: EHVI, EST, EI, in terms of reduction of the Inter-Generational Distance (IGD). However, this was not entirely consistent with change in dimensionality.

[[Diaz-Manriquez et al](https://ieeexplore.ieee.org/stamp/stamp.jsp?arnumber=5949881).] compared four meta-modelling techniques on multiple parameters, and reported that, for MOPs involving 15+ dimensions, Radial Basis Functions, effectively compared to other approximation methods. The same has been reported at multiple instances in literature. However, the GP model was not one of the four compared techniques. Müller created the Surrogate Optimization of Computationally Expensive Multi-Objective Problems (SOCEMO) which uses a combination of local & global sampling strategies. It is a purely surrogate model-based algorithm, doesn’t accelerate any evolutionary algorithm and performs better in high dimensionality. ParEGO [Knowles, 2006] , an extension to the EGO [Jones et al], has a Design and Analysis of Computer Experiments (DACE) model [[Sacks et. al](https://projecteuclid.org/download/pdf_1/euclid.ss/1177012413)] at its base that creates a GP model of the search space.

1. Methods
   1. Differential Evolution

The DE algorithm was introduced in 1997 by Storm & Price, and since then, it has been used very extensively for optimizing complex multi-objective systems. The Differential Evolution algorithm has been proven to be better than similar population-based algorithms such as the Particle Swarm Optimization (PSO) [] and similar EAs [10.1109/CEC.2004.1331139]. The Non-Dominated Sorting DE algorithm used for comparison in this text, comprises of the following actions:

1. *Initialization* of population using latin hypercube sampling
2. *Mutation*
3. *Crossover* using the rand/1/bin strategy
4. *Selection*

(Steps ii to iv are repeated until convergence or exhaustion of evaluation budget)

* 1. Gaussian Process Model

A Gaussian process (GP) model is a probabilistic, non-parametric model which allows uncertainty evaluations on predictions being based on the principles of Bayesian probability. The underlying gaussian process is basically a collection of random variables following a joint distribution of the multivariate normal(gaussian) form.

* 1. The NSDE-GP

1. Evaluation Methods

This section explains the performance evaluation of the NSDE-GP algorithm against some competitive optimization algorithms, the various test optimization problems they were applied to, and the techniques and parameters considered for performance comparison.

* 1. Test Function Suite

The algorithms were tested on following configurations of the problems:

|  |  |  |  |
| --- | --- | --- | --- |
| *Test Problem* | *Number of Objectives* | *Number of Variables (input dimensions)* | *Other Relevant Constants* |
|  |  |  |  |
| DTLZ1 - 7 | 2 | 10, 30 | - |
|  |  |  |  |
| ZDT 1 - 4, 6 | 2, 3 | 10, 30 | - |
|  |  |  |  |
| WFG1 - 9 | 2, 3 | 10, 30 | k = 2, when number of objectives = 2  k = 2\*(number\_of\_objectives – 1), when number of objectives > 2 |
|  |  |  |  |

The NSGA-III algorithm was tested for the above problems in the following configuration:

*Population Size*: P,

*Number of Generations*: 50, such that P\*50 is the evaluation budget, wherever considered,

*Crossover Probability:* 0.30

*Mutation Probability:* 1/number\_of\_variables

* 1. Performance Comparison Parameters:
* Hypervolume: The hypervolume between the first non-dominated front and the origin as the reference point, is calculated at the end of exhaustion of evaluation budget.
* Inverted Generational Distance(IGD):
* Spacing (Pareto) & number of non-dominated solutions:
* Duration of optimization sequence & number of actual evaluations

1. Results
2. Discussion & Scope
3. Acknowledgement
4. References
5. Deb, K., & Jain, H. (2014). An Evolutionary Many-Objective Optimization Algorithm Using Reference-Point-Based Nondominated Sorting Approach, Part I: Solving Problems With Box Constraints. *IEEE Transactions On Evolutionary Computation*, *18*(4), 577-601. doi: 10.1109/tevc.2013.2281535