

# Studying Compartmental Models Interpolation to Estimate MOEAs Population Size

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## ABSTRACT

Dynamical compartmental models capture the population dynamics of Multi-objective Optimization Evolutionary Algorithms. In these models, solutions at each generation are classified in compartments according to Pareto dominance. The size of each model compartment is affected by the other components and changes throughout the generations. Once the dynamics are learned, given the composition of each compartment for the initial population, the model can predict their changes in future generations. In this work, we use these models to select an appropriate population size for a given budget of fitness evaluations. We first learn models parameters for a subset of population sizes and then extract new models from existing ones by spline interpolation. The proposed method allows the investigation of population sizes in-between the ones for which data is available. We verify the proposed method using MNK-Landscapes with twenty bits and one epistatic interaction, running the Adaptive  $\epsilon$ -Sampling  $\epsilon$ -Hood MOEA on several population configurations.

## CCS CONCEPTS

• Theory of computation → Evolutionary algorithms;

## KEYWORDS

Empirical study, Working principles of evolutionary computing, Genetic algorithms, Multi-objective optimization

### ACM Reference Format:

Hugo Monzón, Hernán Aguirre, Sébastien Verel, Arnaud Liefoghe, Bilel Derbel, and Kiyoshi Tanaka. 2019. Studying Compartmental Models Interpolation to Estimate MOEAs Population Size. In *Proceedings of the Genetic and Evolutionary Computation Conference 2019 (GECCO '19)*. ACM, New York, NY, USA, 2 pages. <https://doi.org/10.1145/3319619.3321985>

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GECCO '19, July 13–17, 2019, Prague, Czech Republic

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ACM ISBN 978-1-4503-6748-6/19/07...\$15.00

<https://doi.org/10.1145/3319619.3321985>

## 1 INTRODUCTION

In this work, we aim to study whether our dynamic compartmental models can be applied to algorithm configuration. To verify this concept we use a model that tracks Pareto Optimal (PO) solutions appearance in the population and can compute the total number of PO solutions found by the algorithm, which can be used to evaluate performance [3]. Let us define Function Evaluations (FEs), which is the product of population size by the number of generations. By changing the population size we allow the algorithm to run fewer or more iterations. Since every model is related to population size, we can use them to estimate how performance changes with FEs. With these models, we want to select an appropriate population size for a given budget. We start with deciding a range to explore and create models for a subset of population sizes. Then using spline interpolation we extract new models by interpolating the model parameters. This allows us to only run the algorithms on part of the range, and use the interpolation to fill in the sizes in between the samples, therefore still exploring several population sizes.

## 2 METHODOLOGY

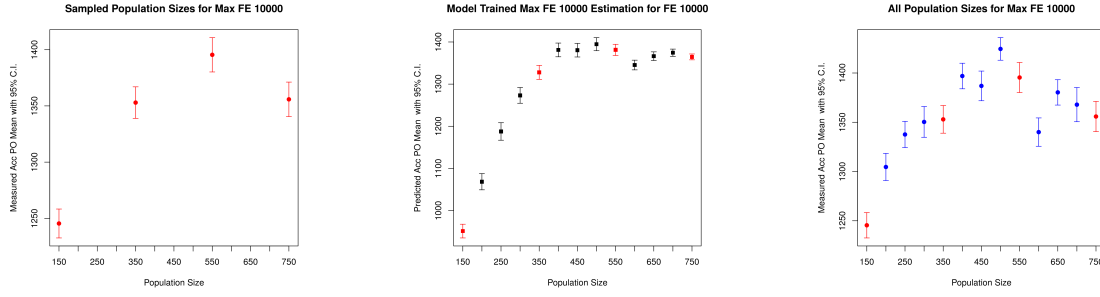
### 2.1 Dynamic Compartmental Models

The model splits the population into three non-overlapping compartments. At generation  $t$ ,  $x_t$ ,  $y_t$  and  $z_t$  represent the population proportion that belong to each compartment which should fulfill  $1 = x_t + y_t + z_t$ . Expressing them in a time-discrete manner would give the following equations:

$$\begin{cases} x_{t+1} = (1 - (\alpha + \beta))x_t + \bar{\alpha}y_t + \bar{\beta}z_t \\ y_{t+1} = \alpha x_t + (1 - (\bar{\alpha} + \gamma))y_t + \bar{\gamma}z_t \\ z_{t+1} = \beta x_t + \gamma y_t + (1 - (\bar{\beta} + \bar{\gamma}))z_t \\ 1 = x_t + y_t + z_t \end{cases} \quad (1)$$

where  $\alpha$  and  $\beta$  are coefficients that represent the loss in  $x_t$  which becomes a gain for  $y_t$  and  $z_t$ , respectively.  $\bar{\alpha}$  and  $\gamma$  represent the loss in  $y_t$  which becomes a gain for  $x_t$  and  $z_t$ , respectively. Finally,  $\bar{\beta}$  and  $\bar{\gamma}$  represent the loss in  $z_t$ . As can be noticed, knowing the composition of the compartments at any generation  $t$  allows the estimation or prediction of their composition at generation  $t + 1$ .

To find the model parameters we pose it as an optimization problem. Setting the function to minimize as the mean square error ( $mse$ ):



**Figure 1: [Budget: 10000 FE] Average Acc. PO over population size. Left: Sampled population sizes used as knots for the spline. Center: Model estimation for the knots and interpolated population sizes. Right: Measured values for all population sizes.**

$\frac{1}{n} \sum_{i=1}^n (D_{est}, D_{meas})^2$  between the  $D_{est}$  estimation produced with current parameters and  $D_{meas}$  the measured values, where  $n$  is the number of observations. This problem is solved using the Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES).

## 2.2 Models by Interpolation

Our models are composed of six parameters ( $\alpha, \beta, \gamma, \bar{\alpha}, \bar{\beta}, \bar{\gamma}$ ), which values differ depending on the population size, algorithm and problem. To interpolate them, we construct a spline for each parameter, taking as data points the pair of population size and parameter value. In this work we want to explore the range [150,750] with {150, 350, 550, 750} as sample population sizes, that act as knots for the spline. New models are generated at intervals of 50, exploring 3 new population sizes between the ones selected as samples.

## 3 ALGORITHM AND TEST PROBLEM

The data to generate the models was produced by running the Adaptive  $\epsilon$ -Sampling  $\epsilon$ -Hood (AeSeH)[1] a many- and multi-objective optimizer with its out-of-the-box implementation and recommended parameters. The algorithm was used to solve test problems generated with a scalable test problem generator, MNK-landscapes[2]. Adjusting the parameters of the generator is possible to create instances with a number of objectives ( $M$ ), decision variables ( $N$ ) and interrelations between variables, epistasis ( $K$ ). An instance with  $N = 20$  bits,  $K = 1$  bit and  $M = 5$  objectives was generated. Due to the low  $N$  is possible to find the PO solutions by enumeration, with 14340 PO solutions for 5 objectives. On this instance, the algorithm was run 30 times with population sizes of {150, ..., 750}, in increments of 50. Generation number varies in each case, according to  $Gen_{Max} = FE_{Max}/Pop$ . The maximum number of FE was set to 10000 simulating a limited budget equivalent to 1% of the whole search space ( $2^{20}$  total possible values).

## 4 EXPERIMENTAL RESULTS AND DISCUSSION

We analyze the average number of Accumulated PO solutions at the end of the budget estimated with the fitted models and the models obtained through interpolation and compare them with the actual measured values running the algorithm. In all plots, the error bars show the 95% confidence interval for each mean.

Looking at Figure 1 left and center plots, we see that for all sizes except 150 the fitted model gets very close to the measured average,

in the particular case of 750 is even a little higher. The  $R^2$  for the model used in 150 is under 0.95, which explains the underestimation produced here. Nevertheless, even with such a model as a knot, the trend is still correctly replicated. Now looking to the center and right figures, we see the influence of our first knot, 150, pulling down the estimations of the interpolated models between [150, 350]. Nevertheless, the growing trend is still correctly maintained when compared to the plot for all sizes. In the next interval of [350, 550], we find that the model estimations get closer to the measured results, and also follows the trend detecting that 400 and 500 obtain better values than 450. Finally, in the last interval of [550, 750], the trend is not correctly replicated, as 700 places a bit higher than 650, which according to the right side of the figure should be below. Since the fitted model of 750 actually overestimates a little in this part, it seems to pull the interval making 700 seem a better option. However, the relative position of the knots points is correct, as two of them place higher than 750 as it should be, and neither of the group is higher than the knot on left, 550. Summarizing, is possible to use the extra information from the interpolated models to guide us towards which regions are worth exploring in more detail.

## 5 CONCLUSIONS

We proposed a methodology to use the Dynamic Compartmental Models as a guide to select population sizes for algorithm configuration under a budget. Using interpolation we avoid running the algorithm for all the sizes. This work showed that the methodology can work and opens the door to use these models for algorithm configuration. In future work, we would like to test other interpolation methods that will help to improve the methodology ability to estimate on larger budgets and find guidelines on how population sizes used as sampling could be selected.

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