Evolutionary and Deterministic Methods for Design,
Optimization and Control with Applications to Industrial and Societal Problems
EUROGEN 2005
R. Schilling, W.Haase, J. Periaux, H. Baier, G. Bugeda (Eds)

METAMODEL-ASSISTED MULTI-OBJECTIVE EVOLUTIONARY OPTIMIZATION

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Key words: Multi-Objective Optimization, Evolutionary Algorithms, Metamodel-Assisted Optimization, Radial-Basis Function Networks

Abstract. *The use of surrogate evaluation models or metamodels in multi-objective Evolutionary Algorithms with computationally expensive evaluations for the reduction of computational cost, through controlled approximate evaluations of generation members, is presented. The metamodels assist the Evolutionary Algorithm by filtering the poorly performing individuals within each generation and subsequently by allowing only the most promising among them to be exactly evaluated. Radial-Basis Function Networks with self-organized selection of centers are employed as metamodels, since they prove to possess the good generalization capabilities that Multi-Objective optimization necessitates. The result is a marked improvement of the metamodel-assisted multi-objective Evolutionary Algorithm in both efficiency and robustness.*

1 INTRODUCTION

Real-word problems such as aerodynamic shape designs can be solved using either gradient-based or global search (Evolutionary Algorithms, Simulated Annealing, etc.) methods. In the literature, adequate evidence concerning advantages and disadvantages of both can be found [1]. This paper deals exclusively with Evolutionary Algorithms (EAs). Despite the convenience of using EAs, which can readily accommodate any ready-to-use evaluation software, their utilization in optimization problems becomes prohibitively expensive if a single evaluation is computationally expensive.

A known remedy to the aforementioned drawback is through the use of surrogate evaluation models or metamodels. Metamodels require training and, for this purpose, an adequate set of already evaluated solutions must be available. The metamodel type along with the training set determine its prediction abilities and the training cost. In the context of the so-called metamodel-assisted EAs, the way the metamodels should be employed during the evolution is of particular importance. The first class of metamodel-assisted EAs utilizes a metamodel which is trained in advance, separately from the evolution, after generating the necessary training data. The evolution,which relies on the *off-line* trained metamodel, produces an 'optimal' solution. This needs to be cross-validated and, depending on the associated error, the metamodel might be updated to support a new search cycle [2, 3] and so forth. The second class uses *on-line* trained metamodels and the exact evaluation tool to selectively support the evolution. The metamodel is continuously retrained during the evolution and, thus, it profits of the most recently collected data [4, 5, 6]. A method for employing metamodels as substitutes for the exact model has also been proposed by the authors for single-objective optimization (SOO) problems [7, 8, 9].

A distinguishing feature of this method is the Inexact Pre-Evaluation (IPE) task. With the exception of the very first (usually one to three) generations, which are based on the exact evaluation tool in order to start populating the training set, in any subsequent generation and for each new candidate solution a local metamodel is trained on the available information in its neighbourhood. So, all population members are approximately evaluated using local metamodels and only the most promising among them are then re-evaluated using the exact tool. The latter are, of course, recorded and can be used as training patterns in the forthcoming generations.

In what follows this filtering process of IPE is incorporated into Multi-Objective EAs (MOEAs) and the gain in both efficiency and robustness is demonstrated through appropriate test-cases.

2 FILTERING THE INDIVIDUALS OF A MULTI-OBJECTIVE EVOLUTIONARY ALGORITHM

The purpose of using inexact pre-evaluations is to filter the poorly performing individuals in the population of each generation and to direct only the promising ones to the exact evaluation tool. The implementation of IPE in a MOEA can be abridged to the

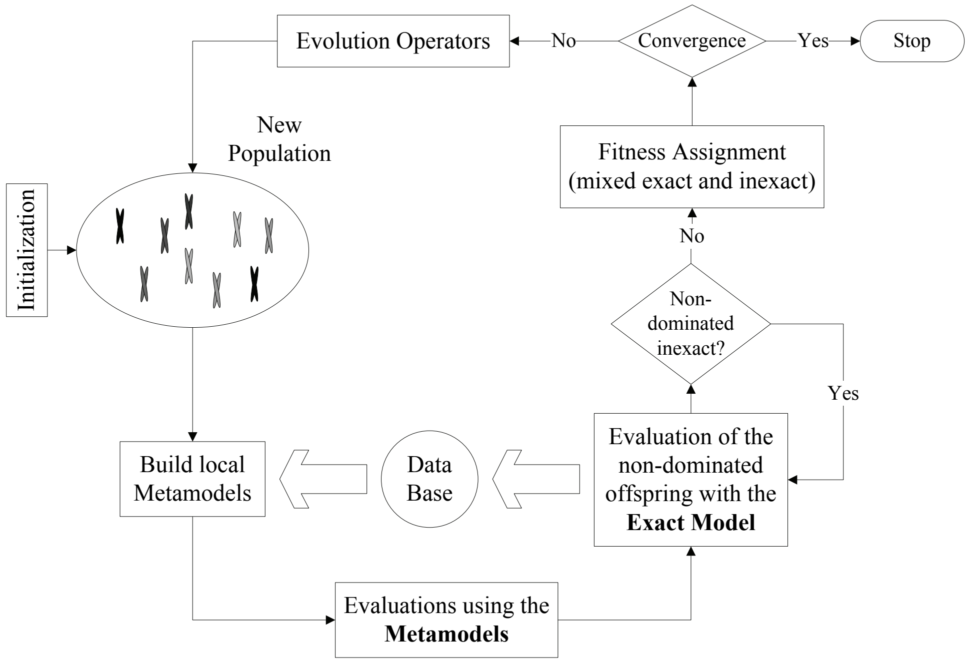


Figure 1: The Inexact Pre-Evaluation in Multi-Objective Evolutionary Algorithms.

following steps (cf. Fig. 1):

Step 1 [Offspring evaluation] In a conventional MOEA, all offspring need to be exactly evaluated. Instead, IPE introduces the following substeps:

Step 1a Evaluate all offspring using locally built metamodels.

Step 1b Evaluate the non-dominated among them with the exact model.

Step 1c If any non-dominated inexactly evaluated individuals still exist and a maximum permitted number of exact evaluations per generation has not been exceeded, repeat from Step 1b.

Step 2 [Evolution] Form the next generation as though it were a conventional EA [10, 11], by indiscriminately treating exact and inexact objective function values:

1. Assign a cost function value to every individual, based on either sharing techniques [12, 13, 14] or the strength concept [15, 16, 17].
2. Update the elit front and apply elitism.
3. Select parents.
4. Recombine parents and mutate their offspring.

Step 3 [Termination] Proceed to Step 1, unless a termination criterion is met.

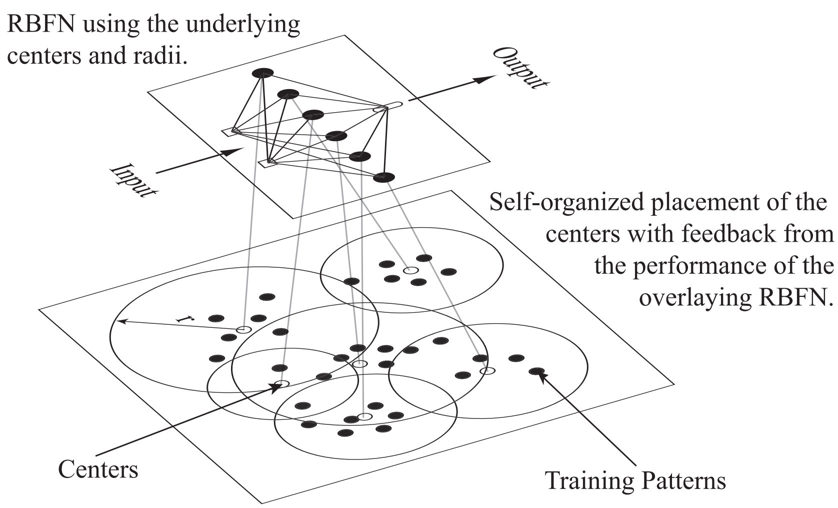


Figure 2: A self-organized Radial-Basis Function Network.

An important point in applying IPE in MOEAs is the selection of the individuals to be exactly evaluated after a pre-evaluation has been obtained, which is not as straightforward as in single-objective EAs. Steps 1a to 1c above imply a loop from which a non-predefined number of exact evaluations per generation results. It depends rather on the approximation error of the metamodels. This scheme is generally more computationally demanding than the one obtained by assigning a provisional cost value by a sharing or strength technique and exactly evaluating a predefined percentage of the best fit individuals [18, 19]. It turns out, however, to be more robust in cases where the metamodels are confronted to a considerable number of failures of the exact evaluation tool. These failures do occur in real-world optimization problems, especially in combination with wide variable ranges, necessary at early design stages, and may be due to severe constraint violations or failures in grid generation, solver convergence etc.

3 RADIAL-BASIS FUNCTION NETWORKS AS PRE-EVALUATORS

The role undertaken by the metamodels in MOO, where a front of non-dominated solutions is sought, is considerably harder than in SOO. The reason lies in the fact that the population remains spread over a relatively extended area of the search domain throughout the evolution [18]. Radial-Basis Function Networks (RBFNs) possess valuable attributes for function approximation [20, 21, 22] and in the context of IPE, by employing local metamodels, they can be trained fast.

In their simple form, however, where they merely interpolate the training patterns, are inadequate for use in MOO. The reason is the poor generalization performance. More elaborate variants can be used instead, which permit a self-organized placement of the RBF centers and subsequently the RBF radii determination. Such variants can be created by coupling RBFNs with Self-Organizing Maps or Growing Neural Gas models [23, 24,

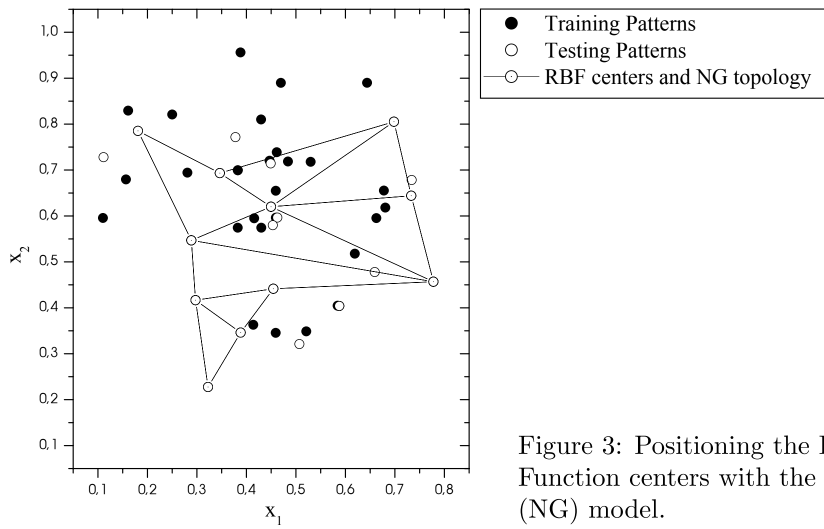


Figure 3: Positioning the Radial-Basis Function centers with the Neural Gas (NG) model.

25, 26, 27] and in what follows will be denoted as *self-organized* RBFNs to distinguish them from the *simple* RBFNs that interpolate the training patterns. The notion of the self-organized RBFN is depicted in Fig. 2. An example of positioning the RBF centers with the Neural Gas model is illustrated in Fig. 3. Note that the RBF centers are not neccessarily placed at the high pattern density areas but where it is needed to improve the RBFN performance, monitored by the testing patterns.

4 APPLICATION IN MULTI-OBJECTIVE OPTIMIZATION

The impact of using metamodels in MOEAs on the computational cost will be demonstrated in the following test-cases, one numerical and one in the field of turbomachinery. The effect of using self-organized RBFNs will be put forward in contradistinction to the use of simple RBFNs as metamodels, in order to stress the importance of the metamodel generalization capability in MOO.

To assess the front quality, the objective space is overlaid with a grid of 200 points per objective. As quality measure of a front, the number of grid points that are not dominated by the front members is used. Apparently, the lower the measure, the better the front.

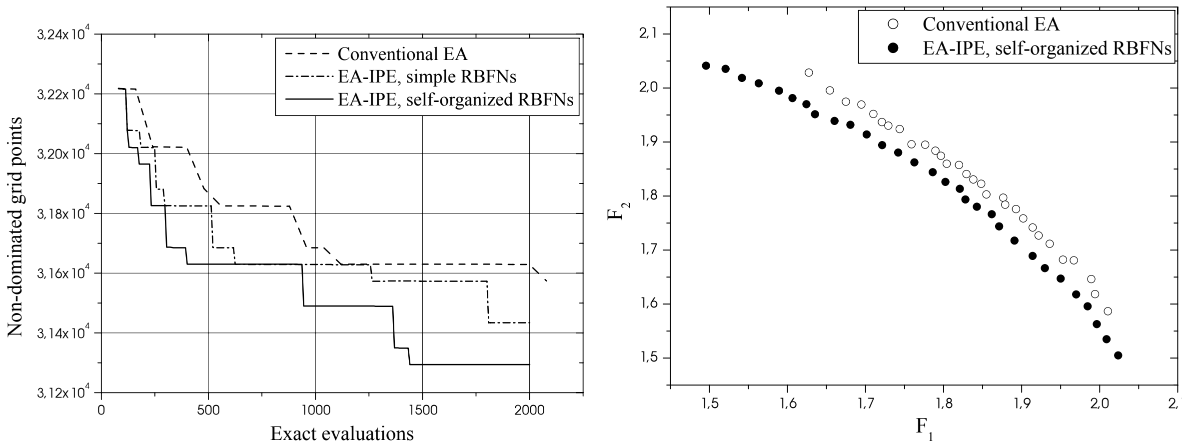
4.1 Numerical example

The first case, defined in INGENET (EU Thematic Network), consists in the minimization of the following multimodal functions:

$$F_j(\mathbf{x}) = \sqrt[4]{\frac{1}{n}\sum_{i=1}^{n}\left\{(x_i - a_j)^2 - 10\cos[2\pi(x_i - a_j)]\right\}}\,, \qquad j = 1, 2$$

with

$$a_1 = 0.0, \quad a_2 = 1.5, \quad \mathbf{x} \in [-5, 5]^n, \quad n = 30$$



(a) Front assessment by counting the non-dominated grid points by each front.

(b) Final fronts of non-dominated solutions.

Figure 4: Numerical example: Convergence history and fronts after 2000 exact evaluations.

The improved performance of the self-organized RBFNs results in more effective filtering of the population individuals within each generation and consequently in higher quality front with the same computational cost as a conventional EA (Fig. 4). Note that the same efficiency is not achievable with metamodels with low generalization capability, such as simple RBFNs (Fig. 4(a)).

4.2 Shape optimization of a compressor cascade

The second case aims at minimizing the total pressure losses of a controlled diffusion compressor cascade airfoil, while maintaining acceptable performance at off-design inlet flow angles. These two confronting objectives have been formulated as the minimization problem of

$$F_1 = \omega_{\beta_{1,\mathrm{DOP}}} = \frac{p_{01} - p_{02}}{p_{01} - p_1}$$

$$F_2 = 10^4 \cdot \sum_{i=1}^{n_{\mathrm{off}}} (\omega_{\beta_{1,i}} - \omega_{\beta_{1,\mathrm{DOP}}})^2$$

where indices $1, 2$ refer to the inlet and outlet planes respectively and DOP to design operating point. n_{off} denotes the number of off-design points examined.

The design operating conditions of the reference airfoil were: $\mathrm{M}_1 = 0.62$, $\beta_{1,\mathrm{DOP}} = 47^{\mathrm{o}}$ and $\mathrm{Re} = 8.41 \cdot 10^5$. Two off-design points were computed for each airfoil design, namely at $\beta_{1,1} = 43^{\mathrm{o}}$ and $\beta_{1,2} = 51^{\mathrm{o}}$. The flow field was computed with an integral boundary layer method (MISES, [28]).

Design variables were the positions of the NURBS control points of the parametrized airfoil, as illustrated in Fig. 5. Geometrical constraints were (a) the max. airfoil thickness

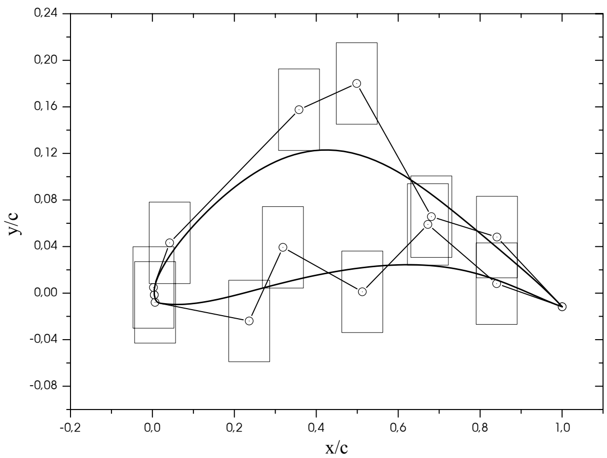


Figure 5: Compressor cascade: The reference cascade profile parametrized with NURBS, along with the bound boxes of the design variables.

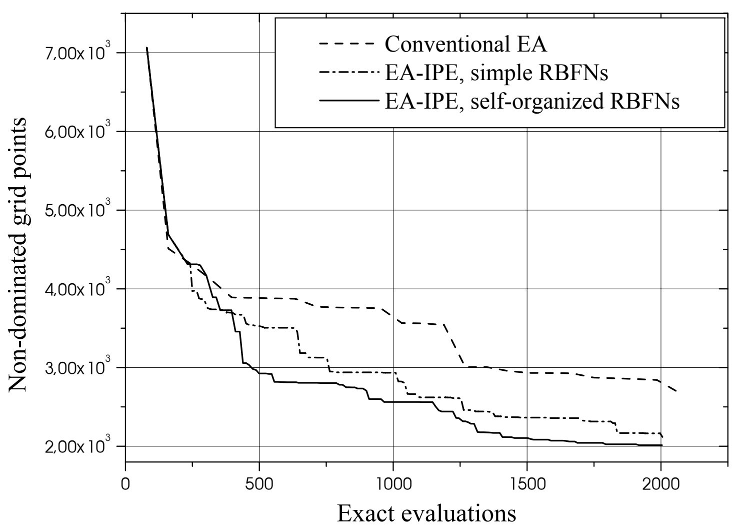


Figure 6: Compressor cascade: Convergence history.

(not less than 10% of the chord), (b) the airfoil thickness at 80% of the chord, (c) the curvature of pressure/suction sides (PS/SS) at the leading edge (LE), (d) the angle between the first PS/SS control points and the LE. Aerodynamic constraint was the flow exit angle β_2, which should be between 19^o and 21^o. All constraints were imposed via penalty function multipliers.

Compared to the previous case, additional difficulties arise due to the numerous constraints and the inability of the flow solver to compute (massively) separated flows, which are likely to occur at off-design conditions. These difficulties result in a high number of failing evaluations; indeed, approximately 350 out of the 2000 evaluations failed. Nevertheless IPE was not inhibited from reducing the computational effort required for a given front quality, as Fig. 6 shows. In Fig. 7 the front obtained from EA-IPE is superposed to the one achieved by a conventional EA and a number of representative solutions belonging to the front are presented.

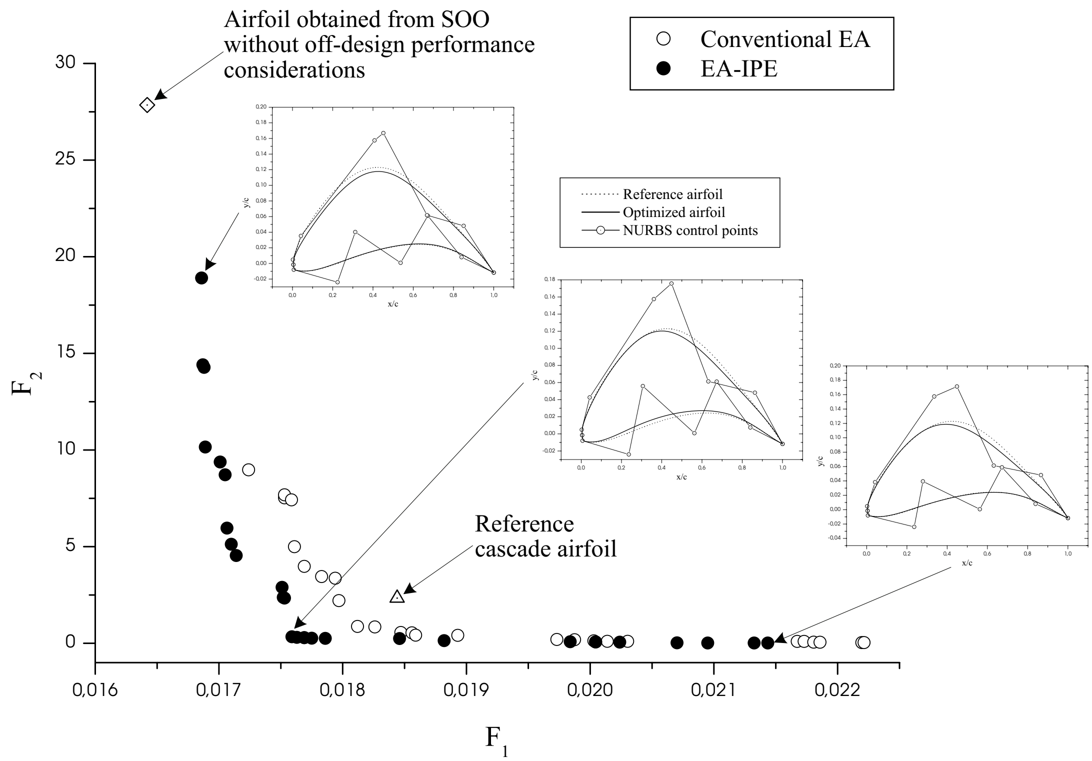


Figure 7: Compressor cascade: Fronts after 2000 exact evaluations and representative solutions obtained by an Evolutionary Algorithm using Inexact Pre-Evaluations.

5 CONCLUSIONS

The use of inexact pre-evaluations through appropriately on-line trained metamodels to single out the promising individuals of each generation, in order only these to be exactly evaluated, increases markedly both the efficiency and the robustness of multi-objective Evolutionary Algorithms. Due to the nature of multi-objective optimization treated with the Pareto front approach, the role undertaken by the metamodels is much harder compared to single-objective optimization. Good generalization properties are indispensable on behalf of the metamodels, and these should be attained by keeping the training cost low. Radial-Basis Function Networks with self-organized selection of centers fulfil this requirement and proved to assist successfully multi-objective Evolutionary Algorithms.

Acknowledgements

This research was sponsored by Dassault Aviation.
The first author was supported by an A.S. Onassis Public Benefit Foundation Scholarship.
The project was co-funded by the European Social fund (75%) and National Resources (25%) — Operational Program for Educational and Vocational Training II (EPEAEK II) and particularly the Program PYTHAGORAS.

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