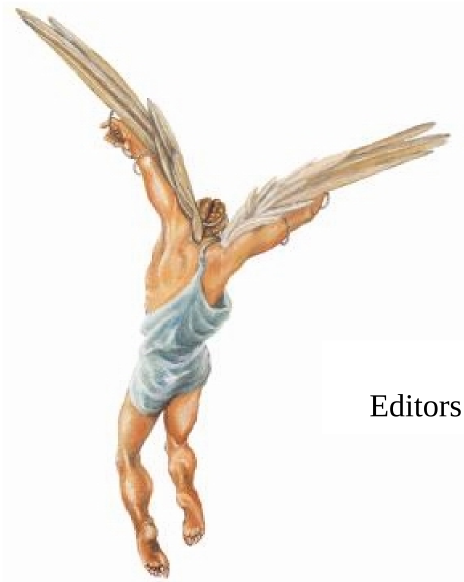

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Metamodel-Assisted Multiobjective Optimization with Implicit Constraints and its Application in Airfoil Design

M. Emmerich
B. Naujoks

University of Dortmund, GERMANY

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METAMODEL-ASSISTED MULTIOBJECTIVE OPTIMIZATION WITH IMPLICIT CONSTRAINTS AND ITS APPLICATION IN AIRFOIL DESIGN

Michael Emmerich, Boris Naujoks

University of Dortmund, Systems Analysis Group,
Dept. of Computer Science,
44221 Dortmund, GERMANY
e-mail:{michael.emmerich, boris.naujoks}@postamt.cs.uni-dortmund.de,

Key words: Airfoil-Design,Metamodel-Assisted Evolutionary Algorithms, Multi-Objective Optimization, Constrained Optimisation, Gaussian field metamodels, Kriging, DACE

Abstract. *This paper proposes new efficient techniques to find (Pareto-)optimal solutions for multiobjective optimisation problems with time expensive evaluations of the objective and constraint functions. These techniques make use of approximate models in order to achieve a faster convergence to the Pareto front. The approximate models - based on Gaussian field metamodels - are capable of self-assessing their local accuracy by means of a confidence measure. The derived methods calculate confidence intervals bounding the values of objective and constraint functions. These intervals are used to pre-screen solutions within a multiobjective evolutionary algorithm (here: NSGA-II). The derived metamodel-assisted methods are extremely useful for tackling optimisation problems in design optimisation, where objective function evaluations are very time consuming. This is demonstrated for a challenging problem from airfoil optimisation - the RAE 2822 problem with three objectives and 10 constraints.*

1 INTRODUCTION

Evolutionary Multiobjective Optimisation Algorithms (EMOAs) are powerful techniques for determining an approximate coverage of the Pareto set for such problems. Recent variants of EMOA are aiming at detecting a good diversity of points on the Pareto set for difficult (discontinuous, multi-modal, high-dimensional) problems. However, they often need a large number of function evaluations to achieve this aim, which sometimes makes these strategies impracticable for problems with time consuming evaluations.

The number of expensive function evaluations can be significantly reduced by replacing precise evaluations partly by fast approximate models for the evaluation of the objective and the constraint functions. This is done in the new metamodel-assisted EMOA (M-EMOA), proposed in this paper.

The proposed variants of M-EMOA incorporate metamodelling into recent versions of EMOA (e. g. NSGA II [1]) by augmenting these EMOA with a pre-screening procedure. Within this procedure search points generated by the variation procedures (mutation, recombination) of the

EMOA are approximately evaluated and it is decided for each of these points, whether it should be rejected or considered for precise evaluation [2].

This paper extends the studies in [2] on the NACA redesign problem. As a new test case for the proposed algorithms the RAE 2822 problem from aerodynamic design has been addressed, which includes three objectives and multiple constraints.

2 GENERAL PROBLEM DEFINITION

Constrained multiobjective optimisation problems in a black-box scenario can be stated as:

$$f_1(\mathbf{x}) \to \min, \dots, f_{n_f}(\mathbf{x}) \to \min, \tag{1}$$

$$\text{s.t. } g_1(\mathbf{x}) \le 0, \dots, g_{n_g}(\mathbf{x}) \le 0, \tag{2}$$

$$\mathbf{x} \in \mathbb{S} := [\mathbf{x}^{min}, \mathbf{x}^{max}] \subset \mathbb{R}^n$$

Here $f_1, \dots f_n$ denote objective functions that are to be minimised and $g_1, \dots, g_m$ denote constraint functions. All functions are considered to be evaluated by means of a time expensive analysis tool, e. g.using CFD and/or FEM/FDM methods, which appear as a black box to the optimisation algorithm.

It is common practise to let the optimisation search for a coverage for the Pareto set (or non-dominated set) of the problem, which is the set

$$M(\mathbb{S}) = \{\mathbf{x} \in \mathbb{S} |\ \nexists \mathbf{x}' \in \mathbb{S} : \mathbf{x}' \prec_p \mathbf{x}\} \tag{3}$$

Here $\prec_p$ denotes the preference relation between solutions, which reads

$$\mathbf{x}_1 \prec_p \mathbf{x}_2, \text{ iff} \tag{4}$$

$$\forall i \in \{1, \dots n_f\} : \ f_i(\mathbf{x}_1) \le f_i(\mathbf{x}_2) \quad \wedge \quad \exists i \in \{1, \dots n_f\} : \ f_i(\mathbf{x}_1) < f_i(\mathbf{x}_2)$$

It is said that $\mathbf{x}_1$ dominates $\mathbf{x}_2$, iff $\mathbf{x}_1 \prec_p \mathbf{x}_2$. This dominance relation can easily be extended to the constrained case by replacing the preference relation $\prec_p$ with an generalised preference relation $\prec_c$:

$$\begin{aligned} \mathbf{x}_1 \prec_c \mathbf{x}_2 \quad :\Leftrightarrow \quad & \mathbf{g}(\mathbf{x}_1) \le 0 \ \wedge \ \mathbf{g}(\mathbf{x}_2) \le 0 \ \wedge \ \mathbf{x}_1 \prec_p \mathbf{x}_2 \qquad \mathbf{or} \\ & \mathbf{g}(\mathbf{x}_1) \le 0 \ \wedge \ \mathbf{g}(\mathbf{x}_2) > 0 \qquad \mathbf{or} \\ & \mathbf{g}(\mathbf{x}_1) > 0 \ \wedge \ \mathbf{g}(\mathbf{x}_2) > 0 \ \wedge \ \text{penalty}(\mathbf{g}(\mathbf{x}_1)) < \text{penalty}(\mathbf{g}(\mathbf{x}_2)) \end{aligned}$$

with

$$\text{penalty}(\mathbf{g}(\mathbf{x})) = \sum_{i=0}^{n_g} \max\{0, g_i(\mathbf{x})\}^2.$$

3 EVOLUTIONARY MULTIOBJECTIVE OPTIMISATION

Recently, many robust techniques for approximating Pareto fronts have been developed that belong to the class of evolutionary algorithms. Among these methods, the NSGA-II Algorithm [1] is commonly used in design optimisation, since it converges comparably fast and it has been extensively tested. Beside this, it is easy to use, since it needs only a few parameters to be specified by the user.

The NSGA-II extends a simple $(\mu + \lambda)$-EA by generalising the sorting procedure in the selection by a sorting procedure for multi-criteria ranking. The sorting used in NSGA-II aims at a *fast convergence* to the Pareto optimal set (promoted by the non-dominated sorting) and a *good coverage* of the Pareto optimal set (promoted by the crowding-distance sorting) [1].

Within a standard $(\mu + \lambda)$-EA, non-dominated sorting and crowded distance sorting are used in order to determine the μ best candidate solutions within the selection (see Figure 1. Non-dominated sorting works in the following way: First the non-dominated set N_1 of a set of candidate solutions G_t is determined. To the elements of N_1 the rank one is given and they are deleted from the set. From the remaining set $G_t \setminus N_1$, again the non-dominated set N_2 is detected and to its members the rank 2 is assigned. Then the non-dominated set from $G_t \setminus (N_1 \cup N_2)$ is determined. This process continues until $G_t \setminus (N_1 \cup N_2 \ldots)$ is empty. Now, each element of the set has a rank. Since multiple candidate solutions may have the same rank for each partition N_i with unique rank i crowding distance sorting can be applied, if it is necessary to determine the μ best solutions. The crowding distance, which is taken as ranking criterion here, assigns a value to each point of the set that is proportional to the coordinate distances to neighbouring solutions measured in the solution space. Elements with a high crowding distance contribute better to a good diversity of the set, and thus are favoured in selection.

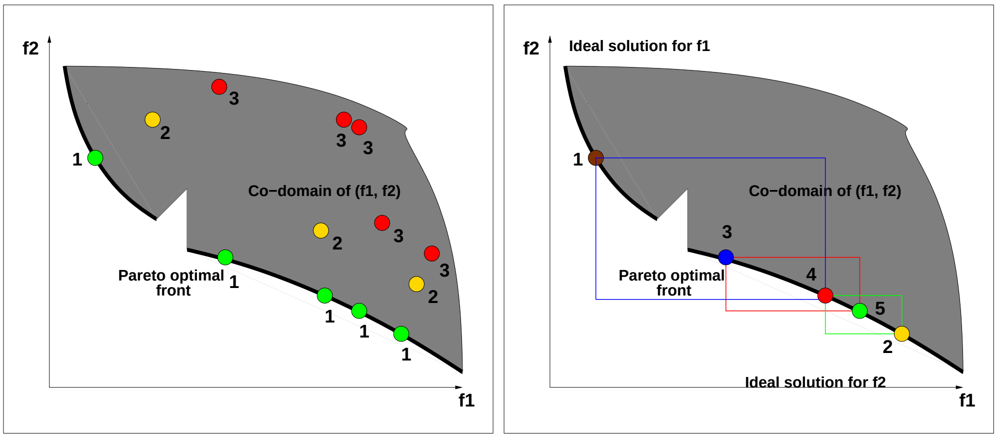

Figure 1: Visualisation of the NSGA-II Sorting Algorithm for a 2-objective problem: The left figure depicts the ranking by means of non-dominated sorting. The numbers attached to the point denote their rank. The right figure visualises the ranking of an partition of non-dominated solutions with unique rank obtained by means of crowding distance sorting. The side length of the rectangles that tangle the neighbouring points in the non-dominated set to a particular point determine the crowding distance of this point, which is used for the ranking.

4 GAUSSIAN FIELD METAMODELS

In order to speed up computation in the presence of time-consuming evaluations approximate evaluators are applied in this work. These approximate evaluators are based on all previous evaluations with the precise model. Since they are 'models of the computer model' they are called *metamodels*. To put things into more concrete terms, a metamodel will be defined as follows:

Suppose we have evaluated a set $\mathbf{X}$ of design points $\mathbf{x}_i \in \mathbb{R}^n, i = 1, \ldots, m$ by means of a precise evaluator y. Then a metamodel $\hat{y} : \mathbb{R}^n_d \to \mathbb{R}$ gives an approximation at each new point $\mathbf{x}_{new} \in \mathbb{R}^n$ by means of interpolating the data in $\mathbf{X}, y(\mathbf{X})$.

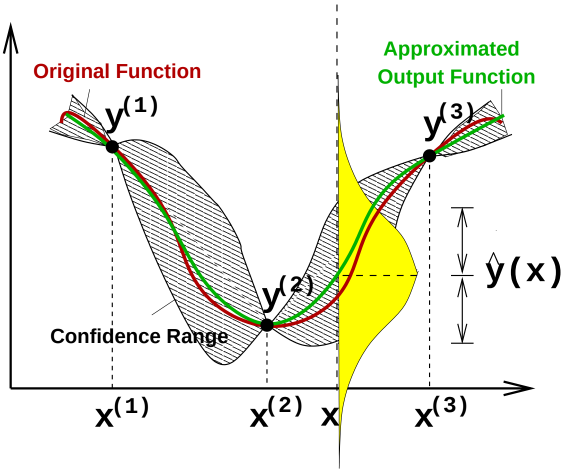

Figure 2: Self-assessing interpolation with a Kriging-metamodel. The original (sinus-)function, the estimated function and its confidence intervals are plotted.

There are several possibilities to do the interpolation, e. g. splines, artificial neural networks, radial basis functions and Shepard polynomials. In this work we decided to use Gaussian random field models, since they do not only provide us with an estimation of the precise value $\hat{\mathbf{y}}(\mathbf{x})$ but also with a confidence measure $\hat{\sigma}(\mathbf{x})$ expressed by the standard deviation of a one dimensional Gaussian distribution (see Figure 2) describing the probability distribution for deviations from the predicted output value under the model assumptions.

The model assumption in Gaussian field models is that the output function y is the realisation of a Gaussian random field $\mathcal{F}$. A Gaussian random field is a set of spatially correlated random variables. More precisely, to each new point $\mathbf{x}_{new} \in \mathbb{R}^n$ a random variable $\mathcal{F}(\mathbf{x}_{new})$ is assigned that is Gaussian distributed with a constant mean value and standard deviation. The correlation between two arbitrary random variables from the Gaussian field $\mathcal{F}(\mathbf{x})$ and $\mathcal{F}(\mathbf{x}')$ is described by a correlation function that depends on the distance between $\mathbf{x}$ and $\mathbf{x}'$, e.g.:

$$c(\mathcal{F}(\mathbf{x}), \mathcal{F}(\mathbf{x}')) = \exp(-\theta|\mathbf{x} - \mathbf{x}'|^2) \quad (5)$$

The parameter θ in this equation is proportional to the smoothness of the Gaussian random field. Moreover, it quantifies how fast the uncertainty about the output of an value grows, when moving away from an precisely evaluated point. Within Gaussian field models this parameter can be estimated from the given sample of points $(\mathbf{X}, \mathbf{y})$. In order to estimate the response at a new point $\mathbf{x}$ the conditional distribution given $\mathbf{X}, y(\mathbf{X})$ can be used:

$$\mathcal{F}_{\mathbf{X},y}(\mathbf{x}) = \mathcal{F}(\mathbf{x})|(\mathcal{F}(\mathbf{X}) = y(\mathbf{X})) \quad (6)$$

```
t ← 0
/* Initialise population P_t ∈ S^μ */
P_t ← init(), D_t = P_t
while t < t_max do
  /* Generate λ solutions by (stochastic) variation operators */
  G_t ← generate(P_t)
  /* Evaluate by metamodel. Choose ν promising solutions */
  Q_t ← pre-screen(G_t ∪ P_t, D_t)
  Q'_t ← evaluate(Q_t)
  D_{t+1} ← D_t ∪ Q'_t
  /* Rank and select μ best */
  P_{t+1} ← select(Q'_t ∪ P_t)
  t ← t + 1
end while
```

Figure 3: Metamodel Assisted Evolutionary Algorithms

The estimate of a value at a new design point $\mathbf{x}$ is now obtained as the mean value $\hat{y}(\mathbf{x}) = E(\mathcal{F}_{\mathbf{X},y}(\mathbf{x}))$ and the estimate of the standard deviation as $\hat{\sigma}(\mathbf{x}) = \sqrt{\mathrm{Var}(\mathcal{F}_{\mathbf{X},y}(\mathbf{x}))}$.

For the calculation of these values[1] the reader is referred to the standard literature [3]. However, it shall be noted that the time to calculate the metamodel from a database with m points lies in the order of magnitude of $\mathcal{O}(m^3)$ and thus can be very inefficient for large point sets. For this reason, in the calculations we performed, we build local metamodels in order to get an estimate for a point $\mathbf{x}$ by training the metamodel only by the $4n$ nearest neighbours of $\mathbf{x}$ in the database and we build a new metamodel for every point that has to be evaluated.

Note that Gaussian field models are also referred to as *Gaussian processes* or as *Kriging models*. While the first term would be more suitable for modelling temporal data instead of spatial data, the latter one also includes some extensions and generalisations for the technique used and thus would be less concise.

5 METAMODEL-ASSISTED EMOA

Two general strategies for integrating metamodels into optimisation may be distinguished. One possibility is to train the metamodel with an initial design of experiments and then optimise on the metamodel. From our experience this procedure does not work very well in high dimensional search spaces, where the quality of global metamodels is low. Instead we use an alternative approach that uses the metamodel to assist an Evolution strategy by pre-screening variants before they are precisely evaluated. This strategy starts working with a global metamodel and then focuses the sampling more and more to a local region of the search space with high performance solutions.

The basic idea in the proposed (local) strategy is to build separate metamodels for the $n_y = n_f + n_g$ response functions $y_1 = f_1, \ldots, y_{n_f} = f_{n_f}$, $y_{n_f+1} = g_1, \ldots, y_{n_y} = g_{n_g}$ and utilise them to pre-screen solutions within a selection procedure of an EMOA. An outline of the basic

[1] provided the mean value and the standard deviation of $\mathcal{F}$ are estimated from the sample

M-EMOA, featuring the $(\mu + \lambda)$-selection, is given in Figure 3:

The algorithm starts by initialising a generation counter t and evaluating an initial population of candidate solutions P_0 obtained by a design of experiments method (here monte carlo sampling was used), which is then fed to the database D of precise evaluation. Then variants are generated from the parent population by means of standard recombination and mutation operators. After this, the most promising solutions are figured out by means of a pre-screening procedure that works with the information provided by the metamodel. The ν most promising solutions are evaluated precisely, fed to the database and are considered in the selection of a subsequent population P_{t+1}. The generational loop closes by incrementing the generation counter t.

It remains to be explicated how the pre-screening with the metamodel is done. Generally the notion of confidence intervals is stressed in order to compare solutions. For each solution an confidence interval located symmetrically around the mean value of prediction is circumscribed for which - under the given model assumptions - it can be said that it contains the true output with a probability of p_α. For independent metamodels for different outputs this can be generalised by

$$p_\alpha = \Pr(\mathcal{F}(\mathbf{x}) \in [\mathbf{y}^-, \mathbf{y}^+]) \tag{7}$$

Symmetrical intervals can be achieved for an output vector $\mathbf{y}$ with an estimation of the mean value $\hat{\mathbf{y}}(\mathbf{x})$ and estimations of standard deviations $\hat{\sigma}(\mathbf{x})$ by choosing an appropriate ω and setting:

$$y_i^- := \hat{y}_i - \omega\hat{\sigma}_i, y_i^+ := \hat{y}_i + \omega\hat{\sigma}_i, i = 1, \dots, n_y \tag{8}$$

The value of ω is determined by the user's choice of p_α in the following way:

$$p_\alpha(\omega) = (1 - 2\Phi(\omega))^{n_y}, \Phi(y) := \frac{1}{2}(1 + \mathrm{erf}(\frac{y}{\sqrt{2}})) \tag{9}$$

This formula stems from the multivariate Gaussian distribution for independent random variables. The figure depicts the relationship between different ω and p_α for different dimensions of the output vector n_y.

Having established interval boxes, we can make comparisons between these boxes. This can be done in the multiobjective case as well as in the constrained case. For two output values the interval boxes can be depicted graphically as it is done in Figure 4 (left) for the example of a two-objective solution space $n_f = 2, n_g = 0$ and for an objective space with one objective and one constraint function in Figure 4 (right).

One pre-screening strategy would now be just to use the mean value of the predictions. By means of this strategy the self-assessment of the metamodel by means of the confidence measure is not used.

An alternative strategy would be to use lower bounds edges of the prediction intervals. This idea is the multiobjective generalisation of the idea of Törn and Zilinskas [6] to use lower bounds instead of precise values for global single criterion optimisation. It has later been used for in metamodel-assisted pattern search by Trosset et al. [5] and for metamodel-assisted evolutionary algorithms by Emmerich et. al [4], both in single-objective optimisation.

This strategy seems more suitable, since it enforces evaluations in unexplored regions but takes also the expected value of the outcome into consideration. The degree regarding the

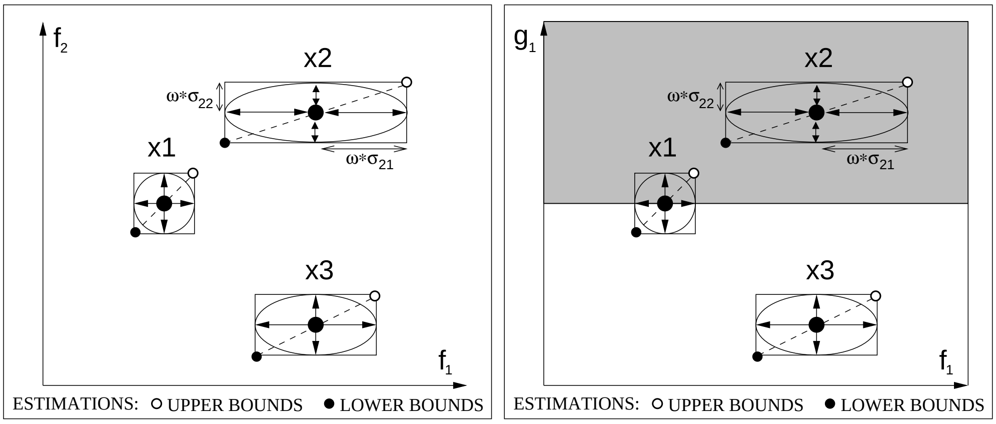

Figure 4: The left figure depict interval boxes for approximations in a solution space with two objectives and the right figure depicts interval boxes for an solution space with a constraint function in an constrained space. Comparing x_1 and x_2 in the first diagram would result in a clear dominance of x_1 to x_2. In the second diagram it is undecided if x_1 dominates x_3, but x_3 dominates x_2 with a probability greater than p_α

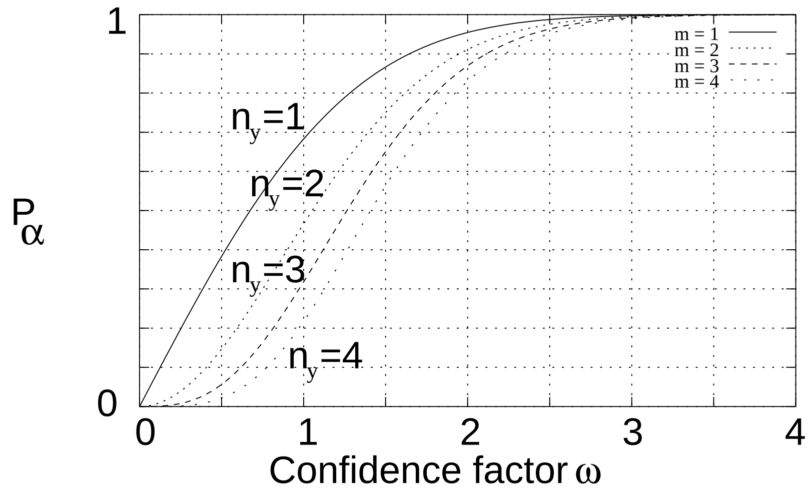

Figure 5: By means of this diagram the confidence factor ω for a desired p_α and a given number of (assumed) independent response functions n_y can be obtained (see equation 9).

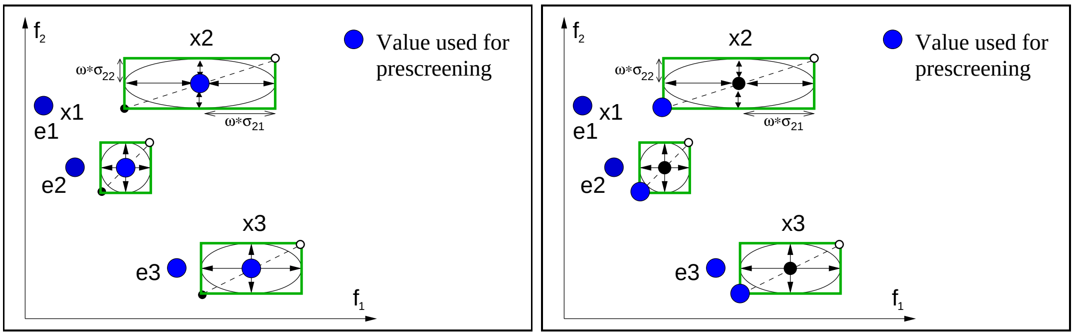

Figure 6: The left figure depicts the pre-screening with the mean values of the confidence intervals and the right figure depict the pre-screening with the lower bounds of the confidence intervals. The big points are the points used within the non-dominated sorting procedure in order to determine the ν best variations.

confidence information can be adjusted by means of choosing ω. However, the choice of $\omega = 2.0$ seems to be suitable. It allows to proceed as well on global as on local optimisation problems ([2], [4]).

6 RAE 2822 AIRFOIL DESIGN OPTIMISATION

The RAE 2822 airfoil is a standard airfoil suggested by the Royal Aircraft Establishment. As in other industries, aircrafts are separated in logical parts for optimisation. This is done, because an optimisation of a whole aircraft design within reasonable preciseness and time is not possible these days. Here, we concentrate on the 2-dimensional design of an airfoil and try to improve it under certain circumstances.

The flow around the baseline design, the RAE 2822 airfoil, is calculated with respect to three different flow conditions, yielding different values for drag, lift and pitching moment for each of the flow conditions. The task is to minimise the drag values C_d^i while not losing lift and keep the pitching moment within a 2 % range. Here $i \in \{1, 2, 3\}$ corresponds to the three given flow conditions, one for cruising and two more off-design conditions. These conditions can be taken from table 1

Table 1: Flow conditions for the RAE 2822 airfoil design problem

	cruise	off-design 1	off-design 2
M	0.734	0.754	0.680
Re	$6.5 \cdot 10^6$	$6.2 \cdot 10^6$	$5.7 \cdot 10^6$
α	2.8	2.8	1.8
transition	3%	3%	11%

The aerodynamic constraints for lift C_l^i and pitching moment C_m^i read:

- $\forall i \in \{1, 2, 3\}$: $C_l^i \geq C_{l,base}$ with $C_{l,base}$ being the lift coefficient of the baseline RAE 2822 airfoil.

- $\forall i \in \{1,2,3\}:$ C_m^i within +/- 2% of the pitching moment $C_{m,base}$ of the baseline RAE 2822 airfoil.

Furthermore, some geometrical constraints have been defined:

- The thickness of the airfoil at 5% should be greater or equal the thickness at 5% of the baseline geometry.
- The maximum thickness should be greater or equal the maximum thickness of the baseline geometry.
- The leading edge radius should be greater or equal 90% of the leading edge radius of the baseline geometry.
- The trailing edge angle should be greater or equal 80% of the trailing edge angle of the baseline geometry.

The geometrical information about a proposed airfoil can be received from the simulation software just after the airfoil shape was generated. The whole time-consuming procedure of solving the flow and all post-processing tasks are not required to receive this information. Therefore, the geometrical constraints are treated differently from the aeronautical ones, which require the costly flow calculation. This different treatment is described in detail later in this paper.

The airfoil parameterisation is done using Bezier weighting points. The y coordinates of these points serve as parameters for the optimisation methods. 3 Bezier weighting points have been in use for both surfaces of the airfoil, resulting in an optimisation problem with 6 degrees of freedom. All other aspects and parameters concerning mesh generation, flow solution, models in use etc. are kept constant during the current investigation.

7 RESULTS

Comparisons on two practical examples (cf. Figure 7, 8 and [2]) from airfoil design demonstrate the gain in solution quality within nearly the same computational time, which can be achieved using the new techniques. By using the metamodel in the EMOA the diversity and the precision of the approximation to the Pareto front can be improved. The results show a further improvement if not only the predicted function value is used but also its corresponding confidence interval. This measure is used by the optimisation method to detect and re-sample insufficiently explored regions of the search space. This has a positive effect on the robustness of the algorithm and on the achieved coverage of the Pareto front.

Considering constrained optimisation the metamodel assistance made it possible to achieve a significantly higher ration of feasible solutions in all five cases of the RAE 2822 problem. Furthermore, it was possible to find an improvement for the baseline design of the RAE 2822 test case. The best feasible solution dominating the baseline design reads $f_1 = 0.022266$, $f_2 = 0.029198$, $f_3 = 0.011615$, with input variables $\mathbf{x} = (-0.000290, -0.000193, 0.000125, -0.000043, 0.000562, -0.000120)$.

Note, that for the RAE 2822 problem, the geometrical constraints, which can be evaluated by a preliminary check which is comparably fast, have been treated in a special way. Solutions have been sampled for several times by the variation operators unless a feasible solution subject to the geometrical constraints has been obtained or the maximal sampling number of 1000 has been exceeded. This has been done in both strategies - the M-NSGA-II and standard NSGA-II - in order to achieve a higher ratio of feasible individuals for the precise evaluation.

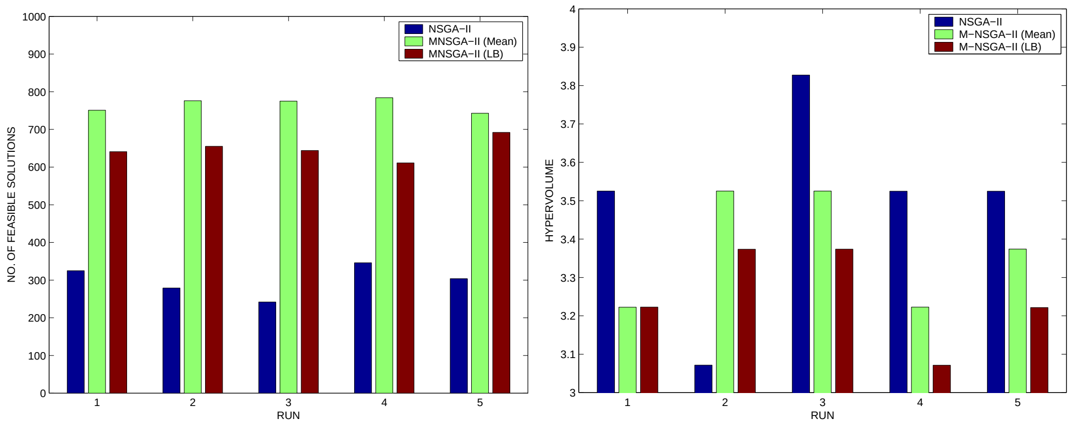

Figure 7: Results for airfoil shape optimisation on the RAE test case. The left figure depicts the number of feasible solutions, i. e. solutions with no constrained violations, obtained with the metamodel assisted NSGA (MNSGA) and standard NSGA and the right figure depicts the volume of the non-dominated region integrated over the interval-box $[0.022, 0.03], [0.028, 0.03], [0.0, 0.04]$ that contains all feasible solution [7].

8 CONCLUSIONS

A metamodel-assisted multiobjective EA has been proposed that is able to tackle constrained multiobjective optimisation problems with time consuming evaluators for the objective and constraint functions. The new idea was to incorporate self-assessing Gaussian field metamodels trained from all previous evaluations, as pre-screening methods into the EMOA method and generalising the search criteria based on lower confidence bounds of the performance from the single criterion case to the multicriterion case. It has been shown how to calculate confidence interval boxes from prediction and confidence information provided by the Gaussian field metamodels about the possible outcomes (functions and constraint values) of the precise evaluation and how to use these interval boxes in the pre-screening of variants suggested by an EMOA.

By means of the new metamodel-assisted NSGA-II it was possible to achieve better solutions for design optimisation problems in airfoil design - namely the NACA redesign problem [2] and the RAE 2822 problem, within the same number of precise evaluations. For the RAE 2822 problem, not only a better variety of Pareto optimal solutions has been obtained, but also solutions that perform better with respect to the 3 different flow conditions.

Moreover, it has been shown that using only the predicted value, instead of a combination of mean value and confidence measure, will likely increase the number of feasible solutions found. But it will not be less sufficient for capturing a large portion of the dominated solution space. An explanation for this is probably that points near the constraint boundaries are more likely to be rejected by a strategy that uses only the information of the predicted value.

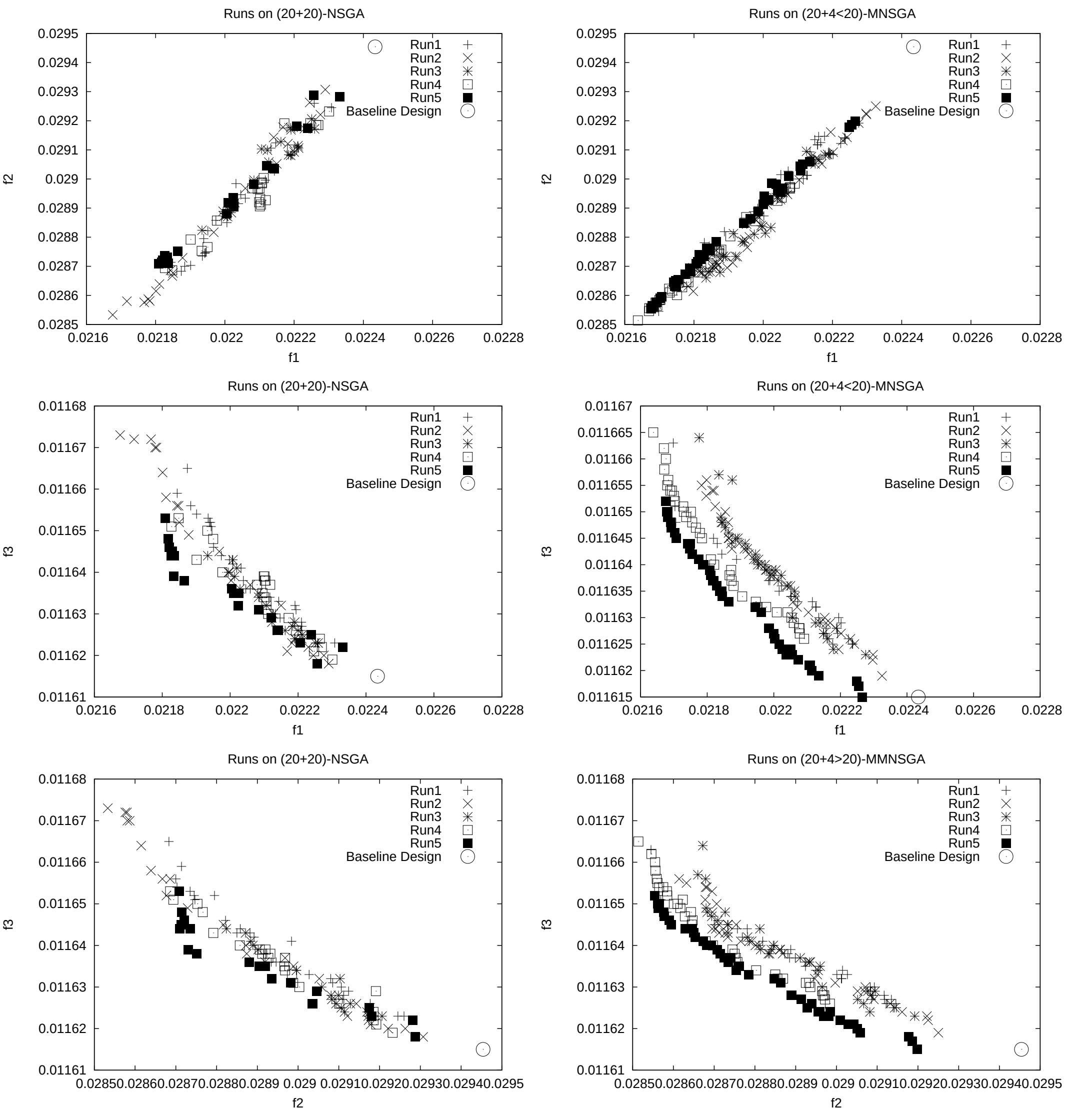

Figure 8: Scatter plot matrix for the 3-objective RAE Airfoil Optimisation. Each plot depicts projections from 3 objective solutions space into a 2 objective subspace. The data points in each particular plot denote Pareto optimal solutions obtained from 5 runs with the same strategy compared with the baseline design.

Further work will have to be done in order to reduce the number of strategy parameters and for comparing the local and global approach to metamodel-assisted multiobjective optimisation. Furthermore, dependencies between different output functions could be modelled (e.g. by means of cokriging models) in order to get more accurate multivariate metamodels.

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