Efficient constraint multi-objective optimization with applications in ship design

Winter, R. de

Appendix B

Appendix

B.1 Expensive Single Objective Optimization

For the optimization of the two single objective ship design problems of Chapter 6 the Modular Adaptive Global Optimization Framework (MAGOF) is introduced. The objective from the two ship design problems were computationally expensive and the constraints are computationally inexpensive. To be ready for more different problem characteristics a modular adaptive framework is proposed. In this appendix a pseudocode and a detailed explanation is presented together with experiments and results on the well known constraint single objective G-Problem suite [93, 61].

B.2 Modular Optimization Framework

The pseudocode of the Modular Adaptive Global Optimization Framework (MAGOF) is presented in Algorithm 4. The evaluation method and strategy are described in more detail in Algorithm 5 and Section B.2.3. The input, the overall explanation of the pseudocode, and the working of the framework are described in more detail in the following subsections.

B.2.1 Input parameters

The input arguments for the modular framework are:

1. **Objective function** $f(\mathbf{x})$ that is to be minimized. The objective function is defined by the user as expensive $f_e(\mathbf{x})$, or inexpensive $f_c(\mathbf{x})$.

2. **Constraint function(s)** $\mathbf{g}(\mathbf{x})$ that consist out of m separate constraint functions, where $m \geq 0$. The constraint function(s) are either defined by the user as expensive $\mathbf{g}_e(\mathbf{x})$, or inexpensive $\mathbf{g}_c(\mathbf{x})$. The constraint functions return the constraint violation, meaning that constraint values $g(\mathbf{x}) \leq 0$ are defined as feasible.

3. **Input space** $x \in \Omega \subset \mathbb{R}^d$ that is limited by the lower and the upper boundary $[\mathbf{x}_{lb}, \mathbf{x}_{ub}]$.

4. **Initial sample strategy and sample size** N_{init} and DoE define how many samples are evaluated in the design of experiments. This should at least be larger than $d+1$.

5. **Evaluation budget** N_{max} defines how many expensive function evaluations are allowed to be evaluated.

6. **RBF strategy domain**, $\Phi = \{Cubic, Gaussian, Multiquadric, InverseQuadratic, InverseMultiquadric, ThinPlateSpline\} \times \{\text{PLOG}, standardized\}$. The RBF strategy domain defines the different surrogates that are used in every iteration to model the computationally expensive functions.

7. **Parallelism** p, is the number of solutions that can be evaluated in parallel. Note that parallelism is not a requirement as p can also be 1.

8. **Acquisition function** α that used to find promising solutions. The acquisition function uses the surrogates or the inexpensive functions directly to find p promising solutions for evaluation.

9. **Constraints first indicator** that defines if the constraints should all be satisfied before the objective function can be evaluated.

B.2.2 Design of Experiments

The framework in Algorithm 4 starts in line 2 by creating a Design of Experiments (DoE). The size and the strategy for the DoE can be chosen by the user and can be random, a latin hypercube sample, solutions on the boundaries, or a Halton sample. Each of these sample strategies has its strengths, however, an empirical comparison by Bossek et al. [23] showed that an as small as possible initial Halton sample [73] is in most cases the most efficient strategy. It is also possible to start with an initial sample that is already evaluated.

Algorithm 4: MAGOF.

Input: Objective function $f(\mathbf{x})$, that can be computationally expensive $f_e(\mathbf{x})$ or computationally inexpensive $f_c(\mathbf{x})$, constraint function(s) $\mathbf{g}(\mathbf{x})$, split where required into expensive constraint function(s) $\mathbf{g}_e(\mathbf{x})$, computationally inexpensive constraint function(s) $\mathbf{g}_c(\mathbf{x})$, decision parameters' lower and upper bounds $[\mathbf{x_{lb}}, \mathbf{x_{ub}}] \subset \mathbb{R}^d$, sampling strategy DoE, number of initial samples N_{init}, maximum evaluation budget N_{max}, RBF strategy domain consisting of 12 RBF strategies $\Phi = \{Cubic, Gaussian, Multiquadric, InverseQuadratic, InverseMultiquadric, ThinPlateSpline\} \times \{\text{PLOG}, standardized\}$, number of solutions that can be evaluated in parallel p, acquisition function α, constraint first indicator c_{first}.

Output: Evaluated solutions.

1 **Function** MAGOF(f, $\mathbf{g}$, $\mathbf{x}_{lb}$, $\mathbf{x}_{ub}$, DoE, N_{init}, N_{max}, Φ, p, α, c_{first}):

2 $\quad \mathbf{x}^* \leftarrow \{\mathbf{x}_1, \cdots, \mathbf{x}_{N_{init}}\} \leftarrow \text{DoE}(\mathbf{x}_{lb}, \mathbf{x}_{ub}, N_{init})$ ▷ Generate DoE, $\mathbf{X} \in \mathbb{R}^{d \times N_{init}}$

3 $\quad \mathbf{F}, \mathbf{G}, \mathbf{X} \leftarrow \text{EVALUATE}(\mathbf{x}^*, f, g, p, c_{first}, N_{init}, \mathbf{F} = [], \mathbf{G} = [], \mathbf{X} = [])$ ▷ Evaluate initial sample and initialize archives $\mathbf{F}$, $\mathbf{G}$ and $\mathbf{X}$

4 $\quad \mathbf{h} \leftarrow \{f_e \cup \mathbf{g}_e\}$ ▷ Union of expensive objective and constraint functions

5 $\quad \varphi^* \leftarrow (\varphi_1, \ldots, \varphi_{|\mathbf{h}|}) \leftarrow (Cubic, standardized)^{|\mathbf{h}|}$ ▷ Initialize RBF strategy for all expensive functions, $\varphi^* \in \Phi$

6 $\quad \mathbf{E}_{i,j} \leftarrow 0 \; \forall (i,j) \in \mathbf{h} \times \Phi$ ▷ Initialize RBF approximation errors for each possible RBF configuration(Φ) for all expensive functions($\mathbf{h}$)

7 $\quad j \leftarrow N_{init}$ ▷ Initialize expensive evaluation counter

8 $\quad$ **while** $j < N_{max}$ **do**

9 $\quad\quad \mathbf{S}^\Phi \leftarrow \left(S_{h_1}^{\Phi_1}, \ldots, S_{h_{|\mathbf{h}|}}^{\Phi_{12}}\right) \leftarrow \{\text{FITRBF}(\mathbf{X}, h, \Phi, \mathbf{x_{lb}}, \mathbf{x_{ub}}) \mid \forall h \in \mathbf{h}\}$ ▷ Fit RBFs using all strategies(Φ) for all expensive functions($\mathbf{h}$)

10 $\quad\quad \mathbf{S}^{\varphi^*} \leftarrow \left(S_1^*, \ldots, S_{|\mathbf{h}|}^*\right)$ ▷ Select best RBF strategy based on line 5 or 15

11 $\quad\quad \mathbf{x}_1^*, \ldots, \mathbf{x}_p^* \leftarrow \text{MAX}(\alpha, p, \mathbf{S}^{\varphi^*}, f_c, \mathbf{g}_c)$ ▷ Get p new solutions based on acquisition function α, use cheap functions f_c and $\mathbf{g}_c$ directly

12 $\quad\quad j \leftarrow j + p$ ▷ Increase iteration counter to new matrix sizes

13 $\quad\quad \mathbf{X} \leftarrow [\mathbf{X}, \mathbf{x}_1^*, \ldots, \mathbf{x}_p^*]$ ▷ Add p new solution vectors, $\mathbf{X} \in \mathbb{R}^{d \times j}$

14 $\quad\quad \mathbf{F}, \mathbf{G}, \mathbf{X} \leftarrow \text{EVALUATE}(\mathbf{x}^*, f, g, p, c_{first}, j, \mathbf{F}, \mathbf{G}, \mathbf{X})$ ▷ Evaluate new solutions

15 $\quad\quad \varphi^*, \mathbf{E} \leftarrow \text{SELECTBESTRBFSTRATEGY}(\mathbf{E}, S^\Phi, \mathbf{F}, \mathbf{G}, \mathbf{X})$ ▷ Update RBF approximation errors $\mathbf{E}$, and new best RBF configuraiton φ^*

16 $\quad$ **end**

17 **return** ($\mathbf{F}$, $\mathbf{G}$, $\mathbf{X}$)

B.2.3 Evaluation of the solutions

On lines 3 and 14 of Algorithm 4 the solutions that are proposed by the DoE, or after optimizing the acquisition function, are evaluated as described in the evaluate Algorithm 5. The approach is dependent on the inexpensiveness of the constraint and objective functions. There are 3 levels of expensiveness. (1) the function can be evaluated almost instantly and can therefore be evaluated millions of times (it must at least be faster than fitting and interpolating an RBF surrogate model). (2) the function requires a little bit of evaluation time and can therefore not be evaluated numerous times and evaluating them millions of times is too costly. Function evaluations of level 2 for example require a few seconds up to a few minutes and are significantly less costly compared to the most expensive evaluations. (3) the function is computationally expensive and the evaluation budget is very limited e.g. computational fluid dynamic simulations or finite element analysis that can take up to hours on a cluster to evaluate.

The inexpensive functions level 1 are used directly in the optimization algorithm, see Section B.2.5. If the constraints are inexpensive level 2, they are evaluated first before the computationally expensive functions. Only if the constraints are satisfied, the expensive functions (level 3) are evaluated. If the constraints are violated, a null is stored instead of the expensive outcome. This way, in the next iteration of MAGOF the RBF surrogates for the expensive functions remain the same as in the previous iteration while for the inexpensive functions level 2 the RBF surrogates are updated.

Algorithm 5: Evaluate.
Input: Solutions $\mathbf{x}^*$ to be evaluated, Objective function $f(\mathbf{x})$, that can be computationally expensive $f_e(\mathbf{x})$ or computationally inexpensive $f_c(\mathbf{x})$, constraint function(s) $\mathbf{g}(\mathbf{x})$, split where required into expensive constraint function(s) $\mathbf{g}_e(\mathbf{x})$, computationally inexpensive constraint function(s) $\mathbf{g}_c(\mathbf{x})$, number of solutions that can be evaluated in parallel p, constraint first indicator c_{first}, objective values of evaluated solutions $\mathbf{F}$, constraint values of evaluated solutions $\mathbf{G}$, evaluated solutions $\mathbf{X}$.
Output: Evaluated solutions.

Function Evaluate($\mathbf{x}^*$, f, $\mathbf{g}$, p, c_{first}, j, $\mathbf{F}$, $\mathbf{G}$, $\mathbf{X}$):
    $\mathbf{G} \leftarrow [\mathbf{G}, \mathbf{g}_c(\mathbf{x}_1^*), \dots, \mathbf{g}_c(\mathbf{x}_p^*)]$ ▷ Add vectors of cheap constraints, $\mathbf{G} \in \mathbb{R}^{m \times j}$
    if not c_{first} **then**
        ▷ If constraints do not need to be satisfied first then add
        $\mathbf{F} \leftarrow [\mathbf{F}, f_e(\mathbf{x}_1^*), \dots, f_e(\mathbf{x}_p^*)]$ ▷ Vector of evaluated objectives, $\mathbf{F} \in \mathbb{R}^j$
        $\mathbf{G} \leftarrow [\mathbf{G}, \mathbf{g}_e(\mathbf{x}_1^*), \dots, \mathbf{g}_e(\mathbf{x}_p^*)]$ ▷ Vectors of evaluated constr $\mathbf{G} \in \mathbb{R}^{m \times j}$
    else
        for $\mathbf{x}_i \in \{\mathbf{x}_1^*, \dots, \mathbf{x}_p^*\}$ **do**
            if $\mathbf{g}_c(\mathbf{x}_i) \leq 0$ **then**
                ▷ If constraints need to be satisfied first
                $\mathbf{F} \leftarrow [\mathbf{F}, f_e(\mathbf{x}_i)]$ ▷ Only add objective value of feasible solutions
                $\mathbf{G} \leftarrow [\mathbf{G}, \mathbf{g}_e(\mathbf{x}_i)]$ ▷ Only add constraint value of feasible solutions
            else
                ▷ If constraints are violated
                $\mathbf{F} \leftarrow [\mathbf{F}, \textit{null}]$ ▷ Don't evaluate and add null
                $\mathbf{G} \leftarrow [\mathbf{G}, \textit{null}]$ ▷ Don't evaluate and add null
        end
return ($\mathbf{F}$, $\mathbf{G}$, $\mathbf{X}$)

B.2.4 Radial Basis Functions

In every iteration of MAGOF, surrogates are fitted to approximate the constraint and objective functions (line 9 of Algorithm 4). However, there are many kernel options and scaling techniques available when fitting RBF surrogates and each option can be good for different scenarios. Therefore, RBF surrogates are fitted with the following kernels: $Cubic$, $Gaussian$, $Multiquadric$, $InverseQuadratic$, $InverseMultiquadric$, $ThinPlateSpline$ and two different scaling strategies are used to scale the constraint and objective values. The standardization method is used so that the uncertainty quantification method can be used for the RBFs. The PLOG transformation from Equation B.1 is selected so that the RBFs can better model steep slopes. For each combination of these kernels and transformation methods, a surrogate is fitted which results in a total 12 RBF surrogate models per expensive function. In every iteration, the RBF strategy with the smallest approximation error is selected (line 5 and 15 of Algorithm 4) and the RBF approximation errors are stored.

$$\textsc{Plog}(y) = \begin{cases} +\ln(1+y), & \text{if} \quad y \geq 0 \\ -\ln(1-y), & \text{if} \quad y < 0 \end{cases} \tag{B.1}$$

B.2.5 Acquisition Function Optimization

The acquisition functions integrated into the framework are: the expected improvement acquisition function [85], the generalized expected improvement acquisition function [119] for parallel evaluations when $p > 1$, and the purely exploitative acquisition function that predicts the objective value with the RBF surrogate without uncertainty. This acquisition function is optimized with the COBYLA algorithm [120]. COBYLA is a single objective optimization algorithm that optimizes an optimization problem with constraints by linearly approximating the acquisition function and the most violated constraint in a small trust region. COBYLA finds the most promising solution in this trust region, then checks the constraint and objective values, and iteratively adjusts the trust region until the trust region is so small and the local optimum is found.

For the functions with expensiveness levels 2 and 3, COBYLA is instructed to use the surrogate models when optimizing the acquisition function. The inexpensive functions (level 1) that can be calculated instantly, are directly used by COBYLA when optimizing the acquisition function. The usage of the inexpensive functions is beneficial because they don't make approximation errors that surrogate models make.

Note that during the optimization of the acquisition function, the inexpensive functions (or surrogate for expensive functions) are evaluated many times.

Because COBYLA is a local optimizer, the COBYLA algorithm starts searching from multiple random locations. This makes it more likely that the global optimum is found.

B.3 Experiments

For this algorithm, four types of experiments are conducted. All experiments are conducted on the G-problem test suite [93, 61].

B.3.1 G-Problem experimental setup

The G-Problems (G1 to G11 from [93, 61]) are selected as an artificially created benchmark suite to validate the performance of MAGOF. A Python implementation of the G-Problems is taken from the CEC 2006 Special Session on Constrained Real-Parameter Optimization [63]. The G-problems considered have between 1 and 9 constraints and between 2 and 20 decision parameters, and all are to be minimized. The optimal solutions are known for all G-problems, some problems have active constraints at the optimum, while other optima are somewhere in the feasible region. The feasibility ratio of the G-Problems varies between less than 1% feasible and 99% feasible per test problem. More details regarding the G-Problems can be found in e.g. [13, 93, 61]. Evaluation of the constraint and the objective functions of the G-problems are computationally inexpensive. However, for the experiments, it is assumed that the objectives are computationally expensive to evaluate.

To test the functionality of the mixed expensiveness, four different configurations of MAGOF are tested with different infill criteria and different inexpensive function handling techniques.

1 Traditional The "traditional" configuration uses MAGOF without any special treatment and/or separation of expensive versus inexpensive functions. The objective and constraint methods are considered equally expensive which in MAGOF means that in every iteration the RBFs are fitted for the constraints and objective, the best RBF strategy is selected, and then the default acquisition function is optimized. The resulting solution is computed and evaluated with the constraints and the objectives.

2 Constraints First: The "constraints first" configuration of MAGOF utilizes the adjustment in the evaluation strategy as presented in Algorithm 5. In this configuration it is assumed that the constraints evaluations are computationally way less expensive compared to the objective evaluation. In every iteration, the RBFs are fitted, the best RBF strategy is selected, and the default acquisition function is optimized using the surrogates. The solution that is proposed is now evaluated first on the constraints. In case any of the constraints are violated, the objective function is not evaluated and the next iteration starts. In case the constraints apply the objective function is evaluated.

3 Constraints Integrated: The "constraint integrated" configuration in MAGOF is not conventional as instead of fitting RBFs for the constraints, the constraints are directly used when optimizing the acquisition function because it is assumed that the constraint function evaluations are computationally cheaper than fitting an RBF and making predictions with RBFs. The RBFs are now only used to model the objective function since the objective function evaluation is assumed to remain computationally expensive.

4 Parallel: The "parallel" configuration of MAGOF does not assume inexpensive constraints or objectives and therefore uses RBF models to model the assumed expensive constraint and objective functions. After the RBF models are fitted, the best RBF approximation is selected, and the generalized expected improvement acquisition function is optimized. The hyperparameter (g_{EI}) of the acquisition function is set in such a way that one solution proposed by the algorithm is purely exploitative ($g_{EI} = 0$), one is explorative and would be most similar to solutions proposed by the expected improvement acquisition function ($g_{EI} = 6$), and one solution is a balance between exploitative and explorative ($g_{EI} = 3$). This way, the generalized expected improvement acquisition function can be used to propose 3 different solutions. After the solutions are proposed, they are evaluated in parallel with both the objective and constraint functions.

All configurations start with an as small as possible initial Halton sample as a DoE. After the DoE the first 3 configurations are allowed to do a total of $300 - |\text{DoE}|$ iterations for the non-parallel configurations. The configuration that proposes 3 solutions per iteration was allowed to do an additional 100 iterations. This way each algorithm configuration has in theory the possibility to do 300 objective function evaluations. Note that the configuration with constraint first, does not necessarily use all these 300 objective evaluations since in the 300 iterations, this configuration also sometimes proposes infeasible solutions. The constraints integrated configuration uses a lot more constraint function evaluations since when optimizing the acquisition function, the constraints are evaluated many more times.

B.4 Results

In Table B.1 the results are presented for the G-problem test suite. In this table, the mean smallest objective scores of the feasible solutions are presented after 10 independent runs of MAGOF with the four different options. Besides the mean objective score, the number of required function evaluations is reported that was required to reach the minimum. Please refer to [63] for the complete set of minima for all functions. A red cross (x) indicates that the optimum was not found within 300 evaluations.

Function		Traditional	Constraint First	Constraint Integrated	Parallel P=3
G01	fv	-15.00	-15.00	$\mathbf{-15.00}$	-13.54
	fe	28	24	**22**	x
G02	fv	-0.304	-0.304	$\mathbf{-0.383}$	-0.304
	fe	x	x	x	x
G03	fv	-0.000	$\mathbf{-0.089}$	-0.006	-0.000
	fe	x	x	x	x
G04	fv	-30665	-30665	$\mathbf{-30665}$	-30665
	fe	26	19	**11**	111
G05	fv	5126.5	5126.5	**5126.5**	5126.5
	fe	41	12	**10**	x
G06	fv	-6957	$\mathbf{-6959}$	$\mathbf{-6959}$	-6956
	fe	x	x	x	x
G07	fv	24.306	24.306	**24.306**	35.479
	fe	34	22	**21**	x
G08	fv	$\mathbf{-0.096}$	-0.096	-0.096	-0.096
	fe	**13**	30	28	100
G09	fv	680.63	1186.8	**680.64**	1597.8
	fe	240	x	**89**	x
G10	fv	7114.3	7088.6	**7049.3**	9233.1
	fe	x	x	**65**	x
G11	fv	0.7500	**0.7500**	**0.7500**	0.7500
	fe	7	**5**	**5**	12

Table B.1: The mean minimum encountered objective score of feasible solutions (fv), and the mean objective function evaluations (fe) required to find the optimal value (a x indicates the known optimal value was not reached in 300 iterations). Four different approaches are compared, the traditional optimization technique, the constraint first approach, the constraints integrated into the acquisition function optimization process, and the approach with the generalized expected improvement acquisition function that proposes 3 solutions in parallel. The best combination of fv and fe are marked in **bold** per G-problem. All G-problems are optimized in 10 independent optimization runs.

Inspection of the results shows that in the majority of the problems using the cheap constraints directly in the optimization algorithm when optimizing the acquisition function is beneficial in terms of execution time and convergence. The other option where the constraints are first evaluated to check for feasibility before the objective function is evaluated also shows better results compared to the conventional approach where the objective is evaluated together with the constraints. The option to propose 3 solutions in parallel with the generalized expected improvement acquisition function does not show good results. It was expected upfront that when proposing multiple solutions for parallel evaluation (and this way save computation time), the number of iterations of the algorithm could be reduced. However, the number of required iterations and therefore also the number of function evaluations is higher compared to the other approaches.

On the G08 test problem, the traditional approach finds the optimum in less required objective evaluations compared to the other approaches. It is assumed that the reason for this quick convergence is that the information gathered from the evaluated infeasible solutions is of great value for this optimization problem. The information from the infeasible evaluated solutions is missing when the constraint first configuration or constraints integrated configuration is used in MAGOF.

B.5 Conclusion and Future Work

Specifically for the optimization of the two single objective ship design problems from Chapter 6, the Modular Adaptive Global Optimization Framework (MAGOF) is introduced. MAGOF can solve constraint single objective problems with a mix of computationally expensive and computationally inexpensive constraint and objective functions. MAGOF uses RBF surrogates for expensive functions, the inexpensive functions can directly be used when searching for promising solutions with an acquisition function. Besides this, a strategy is added to MAGOF that enforces the feasibility of the inexpensive constraints before computationally expensive objective and/or computationally expensive constraints are evaluated. MAGOF with the inexpensive constraints used directly when optimizing the acquisition function showed to be the most promising option when optimizing the G-Problem test suite.

In the future, more research is required on how to effectively propose multiple solutions in parallel with other batch acquisition functions described in e.g. [67, 171, 8]. Secondly, more research is required on setting up the parameterization of optimization problems.

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