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On continuation methods for non-linear bi-objective optimization: towards a certified interval-based approach

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Abstract The global resolution of constrained non-linear bi-objective optimization problems (NLBOO) aims at covering their Pareto-optimal front which is in general a one-manifold in $\mathbb{R}^2$. Continuation methods can help in this context as they can follow a continuous component of this front once an initial point on it is provided. They constitute somehow a generalization of the classical scalarization framework which transforms the bi-objective problem into a parametric single-objective problem. Recent works have shown that they can play a key role in global algorithms dedicated to bi-objective problems, e.g. population based algorithms, where they allow discovering large portions of locally Pareto optimal vectors, which turns out to strongly support diversification. The contribution of this paper is twofold: we first provide a survey on continuation techniques in global optimization methods for NLBOO, identifying relations between several work and usual limitations, among which the ability to handle inequality constraints. We then propose a rigorous active set management strategy on top of a continuation method based on interval analysis, certified with respect to feasibility, local optimality and connectivity. This allows overcoming the latter limitation as illustrated on a representative bi-objective problem.

Keywords Non-linear bi-objective optimization · Continuation · Interval analysis · Constraints activity

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1 Introduction

Non-linear (constrained) bi-objective optimization (NLBOO) is the problem of simultaneously optimizing two criteria and can be formally defined as:

$$\begin{bmatrix} \min & f(x) \\ \text{s.t} & g(x) \leq 0 \text{ and } h(x) = 0 \\ & x \in \mathbb{R}^n \end{bmatrix} \tag{1}$$

with $x \in \mathbb{R}^n$ the decision variables, $f : \mathbb{R}^n \to \mathbb{R}^2$ the two objective functions, $g : \mathbb{R}^n \to \mathbb{R}^p$ inequality constraints and $h : \mathbb{R}^n \to \mathbb{R}^q$ equality constraints. Functions f, g and h can be non-linear.

The feasible region $\mathcal{X}$ is the set of decision vectors that satisfy all the constraints, i.e., $\mathcal{X} := \{x \in \mathbb{R}^n | g(x) \leq 0 \text{ and } h(x) = 0\}$. Its image $\mathcal{F} = f(\mathcal{X})$ in the objective space is called the feasible objective region. A decision vector $x \in \mathcal{X}$ dominates another decision vector y if $f(x) \leq f(y)$ (componentwise) and $f(x) \neq f(y)$. It is called Pareto-optimal if it is feasible and not dominated by any other feasible decision vector. The set of such vectors is denoted $\mathcal{X}^*$, whose image, the Pareto front, is denoted $\mathcal{F}^*$. Intuitively, these solutions correspond to optimal trade-offs between the two objectives. The set $\mathcal{X}^*$ includes the minimizers x_i^* of each individual objective f_i, whose value $f_i^* = f_i(x_i^*)$ is (weakly) non-dominated. The utopia point $f^* = (f_1(x_1^*), f_2(x_2^*))$ is infeasible in general, inducing the necessity of a trade-off. As in single-objective optimization, locally Pareto-optimal vectors can be not global. The global optimization of Problem (1) aims at finding globally Pareto optimal vectors $\mathcal{X}^*$. Local and global Pareto-optimal vectors of (continuous) non-linear bi-objective problems generally form manifolds of dimension 1. This is a major issue for global algorithms, whose diversification aims at both avoiding local optimizers and spreading along these manifolds. The latter can in fact advantageously be handled using continuation methods.

Continuation methods [1] explore step by step a manifold, usually defined as the solution set of an under-constrained system of equations $F(x) = 0$ with $F : \mathbb{R}^{a+b} \to \mathbb{R}^a$, where $b = 1$ for one-parameter continuation considered in the present paper. It has wide applications, e.g. root finding via homotopy [3], nonlinear eigenvalue problems [4], parametric optimization [39], robot path planning [37] and multi-objective optimization (e.g., [22]). Their main limitation for multi-objective optimization is they generally cannot handle constrained problems as constraints induce non-differentiable break points in the followed manifold. Passing those singularities requires their detection and handling constraints activity.

Several certified continuation methods have been proposed: some derive guaranteed step sizes, like [3] based on Smale's α-theory [48], [10] based on interval analysis or [5] based on the reach of a manifold. Others perform rigorous computations using interval analysis and employ solution existence procedures to certify the enclosure of the followed manifold [23,29]. Although more expensive than non-certified methods, they can be used in global optimization algorithms since their cost remains small compared to the price of globality while their rigor is a real advantage, e.g. for enforcing bounds. Continuation alone is however insufficient for the global optimization of Problem (1) since the Pareto front may consist of several disjoint components. It must be coupled with a global optimizer whose role is to attain each component, the continuation role being to cover the attained components. Hence each assume a different aspect of the diversification process.

In this paper, we first survey the use of continuation methods for multi-objective optimization, providing an homogeneous view over several scalarization techniques (Sect. 2), then explaining why implicit parameter continuation based on first-order conditions is preferable

and how it has been used until now. We conclude there is a lack in handling properly inequality constraints and we propose an adaptation of the rigorous continuation method in [29] to this end (Sect. 3), illustrating a possible usage for the global optimization of Problem (1).

2 Survey of continuation approaches for bi-objective optimization

A continuation viewpoint on scalarization methods A common and traditional approach when tackling NLBOO is to transform the problem (1) into a single-objective problem, parameterized such that its optimizers compose a subset of $\mathcal{X}^*$. This process is called scalarization. Scalarization methods generally apply to problems with more than two objectives, though for the sake of clarity we will present them in this context, without loss of generality.

Well-known scalarization methods are the Weighted-Sum (WS) and the ε-constraint (εC), see [7,33]. They induce one additional parameter that control the targeted trade-off in $\mathcal{F}^*$. Capturing a specific trade-off using particular parameters values is not easy, and sometimes impossible. E.g., the weighted sum can not compute solutions whose objective vector is not on the convex hull of $\mathcal{F}$. In order to deal with such limitations, more complex methods have been defined like the Normal Boundary Intersection (NBI) from Das and Dennis [6] and the (Normalized) Normal Constraint (NC) from Messac et al. [30,32]. These scalarization methods introduce a single parameter[1] which corresponds to the dimension of the Pareto frontier of bi-objective problems. Other scalarization techniques using more than one parameter exists: e.g. physical programming [31,49] and directed search domain [9], see also the survey [44]. The extra parameters are used to adapt finely the scalarization in order to capture any Pareto-optimal solutions. In the context of interactive methods [33], scalarization can also be guided by the decision maker through an approximate model of the Pareto-front, see e.g. [19,20].

In the context of global optimization, all these methods have in common that they require solving several instances of the scalarized problem for different parameter values. This problem is clearly related to parametric optimization where a parameter-dependent single-objective optimization problem is solved for different parameter values, the goal being to observe how the optimum vary with respect to the parameters. It is usually supposed that a slight change of the parameters values leads to a slight change of the optimum. Hence, starting from one (globally) computed solution, a basic, but efficient, iterative process is to shift the parameters values and to apply a local solver on the induced new problem, starting from the previously computed optimum (see the discussion in [33, Part II-Introduction] and examples in [6,36]). This iterative process can be seen as a form of continuation which aims at locally approximating the manifold of Pareto-optimal solutions. However, it has several drawbacks. First, being local in nature, the process can easily diverge from the global optimizer of NLBOO. It may be necessary to couple the technique with a global approach, e.g. as in [42]. Second, its performances strongly depend on the selected scalarization and on the local solver. Finally, sampling the parameters values so as to achieve a well distributed sample of Pareto-optimal solutions is not obvious, although several strategies exist see e.g. [8,36].

Another approach in parametric optimization is based on the use of continuation on the system of equations defined by the Karush–Kuhn–Tucker or the Fritz-John first-order conditions [39,41]. The single parameter case can indeed be assimilated to bi-objective optimization, as remarked in [40]. They propose a continuation method based on the WS scalarization of (1) and that implements a strategy for detecting active set change, a required feature to

[1] More precisely, the number of parameters can be reduced to one.

deal with inequality constraints since those changes are singular for the system of first-order conditions. Other singularities can still occur, such as the loss of constraints complementarity, see [28]. Moreover, this method uses second order optimality conditions to track (local) minima of the WS scalarization. Hence, it can not track optimal solutions that are on the non-convex parts of the Pareto-optimal front.

Continuation methods in bi-objective optimization From the work on continuation methods in parametric optimization, Hillermeier [21,22] has proposed a general scheme of continuation approaches for non-linear multi-objective optimization. Although it does not consider inequality constraints, any number of objectives can be used. The process consists of locally tracking the manifold of Pareto-optimal solutions, once a solution is found, implicitly defined by the system of Karush–Kuhn–Tucker first order optimality conditions of (1), defined as follows:

$$F(x,\lambda,r,s) = \begin{pmatrix} \nabla f(x)\lambda + \nabla g(x)r + \nabla h(x)s \\ (\forall i = 1,\ldots,p)\ g_i(x)r_i \\ (\forall i = 1,\ldots,q)\ h_i(x) \end{pmatrix} = 0, \tag{2}$$

with $\lambda \in \mathbb{R}^2_+$, $r \in \mathbb{R}^p_+$ and $s \in \mathbb{R}^q$ ($p = 0$ in [22]). Provided some constraint qualification holds, these conditions are necessary for Pareto optimality (also sufficient in the convex case) with $\lambda \neq 0$, and hence capture all Pareto optimal solutions, see e.g. [2,25]. Uniqueness of the multipliers, which is required for efficiently solving (2), is obtained by additionally adding the normalization equation $\sum_i \lambda_i = 1$ to the system (2). In the bi-objective case, this continuation technique can be viewed as an arc-length continuation. It does not suffer from possible turning points[2] due to a fixed parameter. Hence, the continuation process in [22] is a local technique that takes full advantage of this first-order characterization, but requires an initial Pareto optimal solution. Note that [22] requires also the system to be regular, in particular constraint qualification must hold along the manifold.

One of the first offspring of this scheme is the recovering algorithm of Schütze et al. [46]. Continuation is used as a repair operator inside a global sub-division method. This method sub-divides the search and objective spaces in boxes that are discarded if no solution is found within them. The discarding process is not guaranteed: a box can be removed while it contains Pareto-optimal solutions. The recovering algorithm helps to recover those missing boxes using solutions from neighboring boxes and a continuation process. A similar recovering algorithm is used by Schütze et al. inside a particle swarm optimizer [45]. The aim of the recovering algorithm is here to diversify and improve the spread of the population of the evolutionary metaheuristic. As for Hillermeier [22], this technique has not been applied to problems with inequality constraints.

Harada et al. in [17] have also proposed to combine a metaheuristic with a continuation method. This continuation process, called Pareto Path Following (PPF), is a predictor-corrector algorithm. The predictor step constructs a new solution using the gradient of the objectives as an initial direction of continuation, which is repaired by the Pareto-descent repair operator [18] and a gradient projection method for handling constraints. The corrector step uses the Pareto-descent local search [16]. The authors introduce two new performance measures for bi-objective optimization (but the many-objective case can be easily derived): inter-curve coverage which measures the ability of a method to reach each of the disconnected curves of Pareto-optimal solutions, and intra-curve coverage which measures the spread of solutions on these components. Eventually, a curved-based Genetic Algorithm is

[2] A turning point is somehow a U-turn, where the direction of continuation with respect to the fixed parameter locally changes, hence is singular for this parametrization.

proposed for bi-objective problems. This algorithm considers (locally) Pareto optimal curves as atomic elements of the population. A curve is represented as a cluster of solutions. Genetic crossover operators are applied on solutions from different curves in order to find solutions on non-discovered curves. This method supposes that once a Pareto-optimal solution is found, then all the solutions belonging to the same curve of (locally) Pareto optimal solutions can be obtained by continuation. Hence, the genetic operators focus on inter-curve coverage whereas the PPF focuses on intra-curve coverage. This technique shows better performances at the end of the run than a standard Genetic Algorithm, but it requires more evaluations of the objectives. Although the three objectives and the constrained case are discussed in [17], only one experiment on a bi-objective bound-constrained problem is shown.

As stated in [1], solving a system as (2) by continuation is equivalent to solving a specific system of differential equations. Pereyra [35] has proposed to transform bi-objective unconstrained convex problems into 2-point boundary value problems. In that case, the first-order optimality conditions can be defined as:

$$(1-\lambda)\nabla f_1(x) + \lambda \nabla f_2(x) = 0, \tag{3}$$

with $\lambda \in [0, 1]$. The problem consists of finding the parametric curve $x(\lambda) : [0, 1] \to \mathbb{R}^n$ such that $(x(\lambda), \lambda)$ satisfies (3) for all λ. Since only convex problems are considered, this curve represents the Pareto-optimal solutions. It is computed as the solution curve of the following two-points boundary-value problem:

$$\dot{x}(\lambda) = -H_x^{-1}(x) H_\lambda(x), \quad x(0) = x_1^*, \quad x(1) = x_2^*, \tag{4}$$

where $H_x(x) = (1-\lambda)\nabla^2 f_1(x) + \lambda \nabla^2 f_2(x)$ and $H_\lambda(x) = -\nabla f_1(x) + \nabla f_2(x)$. As for the NBI scalarization, solving (4) requires to find the minimum of each objective x_1^* and x_2^*. The proposed continuation process is a predictor-corrector. The prediction increments the parameter λ by δ_λ, and uses the previous corrected solutions as an initial guess. The correction step is the application of the Newton method on the system (3). This process produces a set of points that covers the Pareto-optimal curve. As the time step parameter is λ, the technique suffers the same drawback of the WS, hence the method is restricted to convex problems. In addition to this continuation method, Pereyra [35] has proposed additional constraints ensuring an homogeneous coverage, in the decision or objective space. A parallel algorithm inspired by the continuation process is also proposed, and shows similarity with NBI. Finally, although the three objectives case is discussed, all these techniques are asserted only on bi-objective problems.

Another method based on solving a system of differential equation by continuation is the method of Potschka et al. [38]. This method is based on the NBI or NC scalarization of (1) in the bi-objective case. More precisely, the considered scalarized problem is as follows:

$$\begin{bmatrix} \min & f_2(x) \\ \text{s.t} & g(x) \leq 0 \text{ and } h(x) = 0 \\ & u^t(f(x) - \hat{f}(v)) = 0 \end{bmatrix}, \tag{5}$$

with $\hat{f}(v) = vf(x_1^*) + (1-v)f(x_2^*)$ and $u = f(x_1^*) - f(x_2^*)$. The parameter v vary within $[0, 1]$. As in [40], an active set of constraints $\mathcal{A}$ is used to handle the change of activity of inequalities. Therefore, active inequalities are considered as equalities, while inactive ones are not considered. Let $h_e(x, v)$ be the additional equality $u^t(f(x) - \hat{f}(v))$. Let $L(x, r_\mathcal{A}, s, s_e, v) = f_2(x) + r_\mathcal{A} g_\mathcal{A}(x) + sh(x) + s_e h_e(x, v)$ the Lagrangian of (5) considering the active set $\mathcal{A}$, with $g_\mathcal{A}$ and $r_\mathcal{A}$ being the vector of active constraints and multipliers, leading to the following first-order conditions:

$$F(x, r_{\mathcal{A}}, s, s_e, v) = \begin{pmatrix} \nabla_x L(x, r_{\mathcal{A}}, s, s_e, v) \\ g_{\mathcal{A}}(x) \\ h(x) \\ h_e(x, v) \end{pmatrix} = 0. \tag{6}$$

Denoting $y = (x, r_{\mathcal{A}}, s, s_e)$, Potschka et al. [38] have proposed to determine the curve of solutions of (6), parameterized by v, solving the following ordinary differential equation:

$$\dot{y}(v) = (\nabla_y F(y, v))^{-1}(\nabla_v F(y, v)). \tag{7}$$

The system is solved by continuation using an integrator applied on the parameter v. The set of active constraints $\mathcal{A}$ is managed such that the process builds feasible and (locally) Pareto-optimal vectors, by using the event detection of the integrator which triggers changes of the active set on conditions similar to [40] (i.e. studying the change of the sign of a constraint or of its multiplier). When a change is detected at a solution x, the active set is updated according to the constraints that are active at x. As in [35], this continuation technique moves along a fixed parameter, here v. Hence, it can stop tracking the curve at turning points when the front is perpendicular to the line connecting $f(x_1^*)$ and $f(x_2^*)$.

One limitation of continuation methods is that they usually require to build the tangent space of the tracked manifold at each iterate. From a system of n equations $F(x) = 0$, the complexity of such an operation is $O(n^3)$. Although the complexity is polynomial, it tends to be very expensive to build tangent space of problems involving thousands of variables. Ringkamp et al. [43] have proposed a tangent space approximation technique in the context of continuation for multi-objective optimization. This technique reduces the complexity of the tangent computation to $O(n^2)$. This approximation method can be applied for any problems where continuation can be used.

Other continuation approaches to multi-objective optimization not based on solving (2) also exist. All the continuation methods presented before requires the use of the gradient (or Hessian) of objectives and constraints. In the case where gradients are not available, Schütze et al. [47] have proposed to use the descent method HCS from Lara et al. [24] in order to perform the continuation on unconstrained multi-objective problems. This technique is based on the observation that, without constraints, there is less chances in finding a direction that improves all objectives at a solution x if this solution gets closer to a (locally) Pareto-optimal front. On the contrary, the chances of finding a direction of trade-off (i.e. that improves one objective and deteriorates the other) increases. The idea in [47] is to build a predictor-corrector technique which uses the HCS to build trade-off directions for predicting new solutions along the Pareto-optimal curve, and to build improving directions for correcting the predicates. The HCS used in [47] constructs these two kind of directions by using gradient approximation techniques. These approximations are also used to determine the length of the continuation step. Although this can, in theory, be used to solve unconstrained problems with any number of objectives, only the bi-objective case is asserted.

Finally, Lovison [26] has studied the global characterization of Pareto-optimal manifolds, through first-order conditions for unconstrained problems. This characterization consists of a piecewise linear approximation of these manifolds using a Delaunay tessellation of the search space, i.e. a decomposition of the search space in simplices. Piecewise linear continuation is used to determine the simplices cut by the manifold. In addition, a process shrinking simplices around the manifold is proposed. The treated problems are unconstrained, but the methods can be adapted to deal with equalities. Any number of objectives can be considered. The technique has some limitations. First, the complexity of the Delaunay tessellation is

exponential with the number of variables, hence the process is limited in problem size. Second, the initial tessellation must be thin enough to guarantee that each connected component of the Pareto-optimal manifold is cut by at least one simplex. Some issues have been partially answered by Lovison [27]. The author indeed proposes a simpler globally convergent version of the algorithm using a decomposition of the search space by regular (equilateral) triangles, dedicated to solve unconstrained problems with 2-variables and 2-objectives. The method shares some similarity with [46]: the former captures the manifold of Pareto-optimal solutions by means of regular triangles, the latter by means of hyper-rectangles.

Conclusion All the techniques presented here show a promising direction towards the design of efficient local methods to use inside a global bi-objective optimization solver. On non-convex problems, methods that fix a priori a parameter to control the continuation, such as scalarization approaches or the fixed parameter continuation, share a common drawback: they are faced to turning points that stop the continuation. While for some advanced techniques the selected parameterization avoids turning points on many problems, in the general case they may cause numerical instability. Note that in parametric optimization, turning points can be treated with jumping strategies, i.e. a jump from the current tracked connected component of solutions to another one using the next parameter value, see e.g. [14,15]. Studying the impact of such strategies in the context of NLBOO is of certain interest. On the other hand, techniques that use an implicit parameterization of the Pareto set, like Hillermeier [21] based on solving (2), naturally avoid such turning points. However, to our knowledge, no such technique in the literature deals with inequality constraints.

3 Certified continuation for constrained bi-objective optimization

Using the certified continuation method [29] for performing the continuation on the first order conditions allows in particular certifying the feasibility, which can turn out to be critical e.g. when feasible vectors are to be used as bounds in a global algorithm. However, neither [29] nor Hillermeier [22] handle active constraints, leading to failure of the continuation process at active constraints change. The correct handling of such change of active constraints allows discovering by continuation larger sets of locally optimal solutions, hence it is critical to be able to perform this in a certified and efficient way. The method also requires the objectives and constraints to be twice continuously differentiable.

In this section, we present an extension of the certified continuation algorithm ParCont defined in [29], to be used on bi-objective problems with correct handling of active constraints change, which is inspired by [40]. This method is based on interval analysis and parallelotope domains. A brief introduction to these notions is given. We refer to [11,34] for more details. This extension handles only the activation (or disactivation) of one single constraint at a time.[3] More than one activation change at the same time is out of the scope of certified numerical methods, and will stop the continuation process in a similar way as e.g. a loss in constraint qualification.

3.1 Preliminaries

Interval analysis and parallelotope domains An interval is a closed connected subset of $\mathbb{R}$. Intervals are denoted by boldface symbols, e.g. $\boldsymbol{x} \subseteq \mathbb{R}$. Lower and upper bounds of an interval $\boldsymbol{x}$ are denoted by $\underline{x} \in \mathbb{R}$ and $\overline{x} \in \mathbb{R}$, with $\underline{x} \leq \overline{x}$, i.e. $\boldsymbol{x} = [\underline{x}, \overline{x}] = \{x \in \mathbb{R} | \underline{x} \leq x \leq \overline{x}\}$. A real

[3] The activation (or disactivation) of k constraints at the same time occurs when the one dimensional curve Pareto frontier crosses the intersection of the k constraints boundaries, which is stable only if $k = 1$.

number x will be identified with the degenerated interval $[x, x]$. A box $\boldsymbol{x} \subseteq \mathbb{R}^n$ denotes a vector of intervals. Interval arithmetic extends elementary operations and functions to interval arguments following the containment principle: any possible real result must be enclosed in the returned interval result. An interval extension of any function can then be defined as its evaluation using interval arithmetic [34]. Interval analysis can be used to solve systems of equations $F(x) = 0$, e.g. interval Newton methods are used to contract an initial box around a solution of the system. Numeric proofs of existence and unicity of solutions are build through an interval Newton operator.

A parallelotope $\widehat{\boldsymbol{x}}$ is the image of a box $\boldsymbol{w}$ through an affine map $w \to Cw + \tilde{x}$. It is defined by a triple $(C, \boldsymbol{w}, \tilde{x})$, where $C \in \mathbb{R}^{n\times n}$, $\boldsymbol{w} \subseteq \mathbb{R}^n$ and $\tilde{x} \in \mathbb{R}^n$, whose corresponding parallelotope is $\widehat{\boldsymbol{x}} = \{Cw + \tilde{x} \in \mathbb{R}^n : w \in \boldsymbol{w}\}$. We call C, $\boldsymbol{w}$ and $\tilde{x}$ the characteristic matrix, box and vector of the parallelotope. The interval hull $\square\widehat{\boldsymbol{x}}$ is easily computed as $C\boldsymbol{w} + \tilde{x}$ using interval arithmetic. Parallelotopes are used in [11] in order to enclose and certify b-manifolds defined by a system $F(x) = 0$, with $F : \mathbb{R}^{a+b} \to \mathbb{R}^a$: interval techniques are applied to the auxiliary system $G(w) = 0$, with $G(w) = F(Cw + \tilde{x})$, whose derivative is $G'(w) = F'(Cw + \tilde{x})C$. The last b components of w are identified to parameters: w is split into $w = (u, v)$ with $u \in \mathbb{R}^a$ and $v \in \mathbb{R}^b$. The aim is to build parallelotopes $\widehat{\boldsymbol{x}} = (C, (\boldsymbol{u}, \boldsymbol{v}), \tilde{x})$ that contain a solution for each parameters values in their domain, i.e. satisfying

$$\forall v \in \boldsymbol{v}, \quad \exists u \in \boldsymbol{u}, \quad G(u, v) = 0. \tag{8}$$

This property expresses that the manifold crosses the whole parallelotope along the parameter subspace. Proofs of this property can be obtained through a dedicated interval Newton method, see [11]. It also proves that the crossed manifold is continuously differentiable.

The certified continuation method parCont In [29], the authors have proposed a certified and interval-based continuation method ParCont. The method constructs by continuation a covering with parallelotopes of a one-manifold, implicitly defined by a system $F(x) = 0$, $F : \mathbb{R}^n \to \mathbb{R}^{n-1}$. The process is certified, i.e. the paving is proved to contain a unique continuous curve of solutions. ParCont can be seen as an intervalization of the arc-length continuation.

ParCont takes as input a system $F(x) = 0$ implicitly defining a one-manifold, an approximate initial solution x_0 on the manifold and a search domain $\boldsymbol{x}^{\text{init}}$. It also considers a direction $d \in \{-1, 1\}$ of continuation that allows performing the continuation in each direction from x_0. ParCont constructs and returns two sequences of parallelotopes $(\widehat{\boldsymbol{x}}_1, \ldots \widehat{\boldsymbol{x}}_K)$ and $(\widehat{\boldsymbol{y}}_0, \ldots, \widehat{\boldsymbol{y}}_K)$. Each parallelotope $\widehat{\boldsymbol{x}}_k$ is built such that it is proved being crossed by a unique solution curve from the input edge $\widehat{\boldsymbol{x}}_k^{in} = (C_k, (\boldsymbol{u}_k, \underline{v}_k), \tilde{x}_k)$ to the output edge $\widehat{\boldsymbol{x}}_k^{out} = (C_k, (\boldsymbol{u}_k, \overline{v}_k), \tilde{x}_k)$. Each parallelotope $\widehat{\boldsymbol{y}}_k$ is a contraction of the output edge of $\widehat{\boldsymbol{x}}_k$, i.e. a tight enclosure of the single solution of the curve in $\widehat{\boldsymbol{x}}_k^{out}$. The exception being $\widehat{\boldsymbol{y}}_0$ which encloses the solution on the input edge of $\widehat{\boldsymbol{x}}_1$. Each iteration k of ParCont builds a parallelotope $\widehat{\boldsymbol{x}}_k$ (and $\widehat{\boldsymbol{y}}_k$) in the direction of continuation and of length h along the manifold, starting from $\widehat{\boldsymbol{y}}_{k-1}$. An iteration k may fail, which induces a reduction of the length of the continuation step h, and the restart of the iteration k. Figure 1 displays several steps of ParCont. Singular solutions along the manifold cannot be certified, hence triggering a failure of the iteration. The step length is decreased accordingly, and therefore the method will conserve toward the singularity in case some are present on the manifold, as illustrated on Fig. 1.

The algorithm stops once the tracked manifold provably (1) exits the search domain $\boldsymbol{x}^{\text{init}}$, (2) loops or (3) the step length h becomes too short. Correctness, termination and asymptotic convergence of the method are proved in [29]. The complexity of one iteration of ParCont

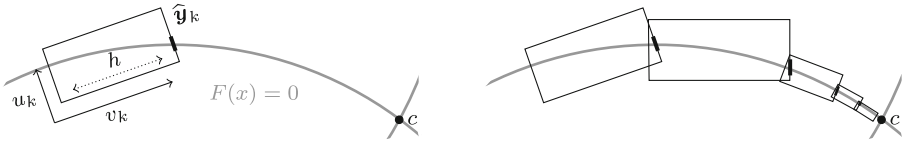

Fig. 1 *Left* A parallelotope $\widehat{\boldsymbol{x}}_k = (C_k, (\boldsymbol{u}_k, \boldsymbol{v}_k), \tilde{x}_k)$ constructed by ParCont. *Right* Successive steps of ParCont. c is a singular point of $F(x) = 0$

is $O(n^3)$. The total number of iterations depends on the length of the manifold within $\boldsymbol{x}^{\text{init}}$ and on the conditioning of F.

3.2 Adapting ParCont to bi-objective optimization

Consider a NLBOO problem as (1) and its system F of first order conditions as (2), involving variables $x \in \mathbb{R}^n$ and multipliers $\lambda \in \mathbb{R}^2_+$, $r \in \mathbb{R}^p_+$ and $s \in \mathbb{R}^q$. We denote by $z = (x, \lambda, r, s)$ the vector of these variables and multipliers, and consider that ParCont iterates on parallelotopes $\widehat{\boldsymbol{z}}_k$. We consider the Fritz John conditions instead of KKT conditions by using the normalization $\lambda^T\lambda + r^T r + s^T s = 1$ (instead of $\sum_i \lambda_i = 1$ for KKT), which are valid regardless of any constraint qualification.

The singularities of F have been analyzed in [28,40] in the case of parametric optimization. The bi-objective first order conditions present the same kind of singularities, e.g. loss of constraint qualification or change in the set of active constraints. The latter occurs at solutions z where there is a constraint i with $g_i(x) = 0$ and $r_i = 0$. The equation $g_i(x)r_i = 0$ actually consists of the product of two zero quantities. Hence, two paths are possible, one where $g_i(x) \neq 0$ and $r_i = 0$ (only the part $g_i(x) \leq 0$ is feasible), the other where $g_i(x) = 0$ and $r_i \neq 0$ (only the part $r_i \geq 0$ is feasible).

Example 1 Consider the bi-objective problem with $f_1(x) = (x_1 + 1)^2 + x_2^2$, $f_2(x) = (x_1 - 1)^2 + x_2^2$ and inequality constraint $g(x) = x_1 - x_2 \leq 0$. Variables of F are here $z = (x_1, x_2, \lambda_1, \lambda_2, r)$. This problem is illustrated in the left hand side graphic of Fig. 2 in the plane (x_1, x_2). The solution $c = (0, 0, \sqrt{2}/2, \sqrt{2}/2, 0)$ is singular for F. The curve of solutions bifurcates at this point in two paths: the path from $a = (-1, 0, 1, 0, 0)$ to $b = (1, 0, 0, 1, 0)$ satisfies $r = 0$ but is infeasible from c to b ($g(x) > 0$); the path from $d =$

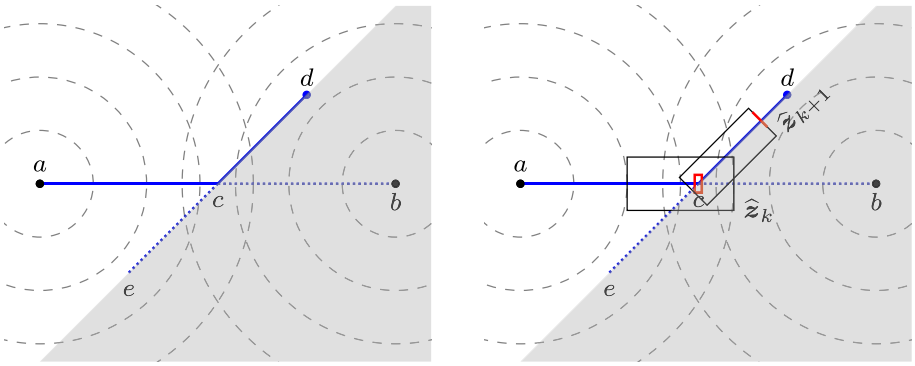

Fig. 2 Bi-objective problem of Example 1

$(0.5, 0.5, 0, \sqrt{2}/2, \sqrt{2}/2)$ to $e = (-0.5, -0.5, \sqrt{2}/2, 0, -\sqrt{2}/2)$ satisfies $g(x) = 0$ but is infeasible from c to e ($r < 0$).

Remark 1 The x-projection depicted in Fig. 2 can be misleading because it hides the multipliers space. In particular, the case where one constraint is activated and another constraint is disactivated at the same x is stable: in fact, two successive different single activation changes occur, separated by a Pareto curve along the multiplier space with fixed x (see Table 1 in Sect. 3.3).

These singularities can be removed by correctly handling subsystems corresponding to active constraints. Given a set $\mathcal{A}$ of active constraints, it is known (see [40]) that applying a continuation on the full system (2) is equivalent to applying it on a reduced system involving only the active constraints:

$$F_{\mathcal{A}}(x, \lambda, r, s) = \begin{pmatrix} \nabla f(x)\lambda + \nabla g_{\mathcal{A}}(x) r_{\mathcal{A}} + \nabla h(x) s \\ (\forall i \in \mathcal{A})\ g_i(x) \\ (\forall i = 1, \ldots, q)\ h_i(x) \end{pmatrix} = 0, \tag{9}$$

with $x \in \mathcal{X}$, $r \geq 0$ and $\lambda \geq 0$, and the normalization equation $\lambda^T \lambda + r^T r + s^T s = 1$. Note that $r_i = 0$ for all $i \notin \mathcal{A}$. As ParCont cannot handle singularities, we apply it on (9) instead of (2), and manage correctly the active set.

Let $\mathcal{A}_k$ be the set of active constraints at iteration k of ParCont, and $\widehat{z}_k = (C_k, (\boldsymbol{u}_k, \boldsymbol{v}_k), \tilde{z}_k)$ a parallelotope certified to contain solutions of (9), i.e. condition (8) holds in $\widehat{z}_k$. In order to maintain a correct active set for the next iteration of ParCont, it is required to determine changes in $\mathcal{A}_k$ that occur on the solution curve contained in $\widehat{z}_k$. To this end, we introduce the following Constraint Satisfaction Problems (CSP) for each constraint g_i:

$$\left[\begin{array}{l} z = C_k(u, v) + \tilde{z}_k,\ \ F_{\mathcal{A}_k}(z) = 0,\ \ \gamma_i(z) = 0 \\ u \in \boldsymbol{u}_k, v \in \boldsymbol{v}_k \end{array} \right], \tag{10}$$

whose variables u and v take their values in $\boldsymbol{u}_k$ and $\boldsymbol{v}_k$ respectively, i.e. the characteristic box of $\widehat{z}_k$. The virtual variables z, and the first constraint, express the transition from the parallelotope basis. The second constraint enforces (9). The third constraint deals with the activation/disactivation of inequality g_i: the function $\gamma_i(z)$ is defined as $g_i(x)$ if $i \notin \mathcal{A}_k$ (i.e. we try to activate g_i), or as r_i if $i \in \mathcal{A}_k$ (i.e. we try to disactivate g_i). Since (8) holds for (9) in $\widehat{z}_k$, there is an unique solution to the equations $F_{\mathcal{A}_k}(z) = 0$ for each $v \in \boldsymbol{v}_k$. Hence, solving (10) can be done by performing an unidimensional search in the domain $\boldsymbol{v}_k$ of variable v, whose complexity is generally low. In addition, since only the first change of activity is of interest, a single solution is computed, the one closest to $\underline{v}_k$.

Changes in the active set must be certified for ParCont to remain rigorous. To this end, we propose to solve (10) with an interval-based Branch and Prune (B and P) method, adapted to the specificities of this problem (i.e. it branches only on the domain $\boldsymbol{v}_k$ of the variable v, and uses only the interval Newton to solve the constraints). For each CSP (10), the method returns either no solution, thus proving no change of activity occurs in $\widehat{z}_k$ for this constraint; or the first encountered certified solution box $(\boldsymbol{u}_k^i, \boldsymbol{v}_k^i)$ identifying a verified change; or the first encountered non-certified solution box if the computational precision is insufficient. The process is applied at each iteration of ParCont, once a parallelotope $\widehat{z}_k$ has been certified. A CSP (10) is build and solved for each potentially inactive/active constraints, i.e. constraints for which $\gamma_i(\square\widehat{z}_k)$ contains 0.

If all of these CSP return en empty solution, then no change occurs in $\widehat{z}_k$ and the iteration of ParCont continues as usual. Otherwise, a set of (certified or not) solution boxes $(\boldsymbol{u}_k^i, \boldsymbol{v}_k^i)$

is returned. Among them, the one non-empty closest to $\underline{v}_k$ is kept. If this solution box is not certified, or if it overlaps an other non-empty solution box $(\boldsymbol{u}_k^j, \boldsymbol{v}_k^j)$, then it is not possible to certify the change of activity: either the numerical precision is not enough or two changes occurs at the same place. Consequently, a failure of the current iterate of ParCont is triggered, and the iteration restarts with a reduced step length h. Otherwise, a change of constraint activity has been reliably identified. The corresponding box $(\boldsymbol{u}_k^i, \boldsymbol{v}_k^i)$ is used to build $\widehat{\boldsymbol{y}}_k$, the output edge parallelotope of $\widehat{\boldsymbol{z}}_k$, and the active set $\mathcal{A}_{k+1}$ for the next iteration can be constructed accordingly. Note that if the activation status of the constraint g_i has changed on the previous step of ParCont then the first solution is the reverse change of activity of this constraint, which must be avoided. In this case, the second change of activity of g_i has to be considered instead of the first. The two parallelotopes built following this procedure are illustrated on the right hand side graphic of Fig. 2.

This strategy for maintaining the correct active set of constraints has been incorporated in ParCont. The stopping criterion of ParCont based on the search domain only considers the domains of λ_1 and λ_2 (i.e. $\lambda_1, \lambda_2 \geq 0$), the non-negativeness of the multipliers r_i being maintained by the active set strategy. Note that the proposed adaptation only deals with singularities of (2) induced by a change of the active set, but other singularities, such as the loss of constraint qualification, cannot be handled.

3.3 Illustrative experiment

ParCont and its adaptation to NLBOO have been implemented in C++ using the RealPaver [13] API, implementing routines such as interval Newton methods and many other constraint solving techniques, and using Gaol [12] for interval arithmetic. This experiment has been run on a computer under Linux Ubuntu version 11.10, with processor Intel i5-2400 3.10 GHz and 4 Gb of RAM. Parameters of ParCont are tuned as prescribed in [29].

We consider the bi-objective problem from [50] with 7 variables and 11 constraints, for the design of a speed reducer. In addition, domains of variables are considered as inequality constraints: constraints are hence denoted $g_i, i = 1 \ldots 11$ and bound constraints $\underline{g}_{x_i}$ and $\overline{g}_{x_i}$ for respectively the lower and upper bound of x_i. There is hence a total of 25 constraints. The Pareto front of this non-convex problem turns out to be connected and even convex, hence scalarization methods would succeed in approximating it. However, it is well suited to the illustration of our method, due to its nonlinearity and the numerous changes in its active constraint set within the front. We apply ParCont starting from the minimizer of f_1, and it takes approximately 0.25 s to produce 58 parallelotopes enclosing the whole Pareto curve. The captured Pareto-front is shown in Fig. 3, where it is depicted as the lines connecting the images of solutions sampled from the computed parallelotopes for the sake of clarity.[4] The points a, b, c and d correspond to solutions on which a change of $\mathcal{A}$ occurs. ParCont starts at solution a and tracks solutions until it reaches d. The obtained solutions show that the constraints $g_7, g_9, \underline{g}_{x_2}$ and $\underline{g}_{x_7}$ are always active. Constraints reported in Table 1 change activity during the process, the others are inactive along the Pareto front.

Consider first the path from a to c. Table 1 shows that 7 constraints, for 7 variables x, are active at its start a. Hence, the active set of constraints form a square system of equations uniquely defining the values of x. In such situation, the Pareto manifold remains constant in x, but moves in the multipliers space $(\lambda, r_{\mathcal{A}})$. The disactivation of $\underline{g}_{x_6}$ is finally observed, allowing the continuation to exit a. On the path $a \rightarrow b$, 6 constraints are active, hence the continuation tracks other solutions in the variable space, and in the objective space. When

[4] Parallelotopes allow a cheap and certified sampling of the Pareto frontier they include.

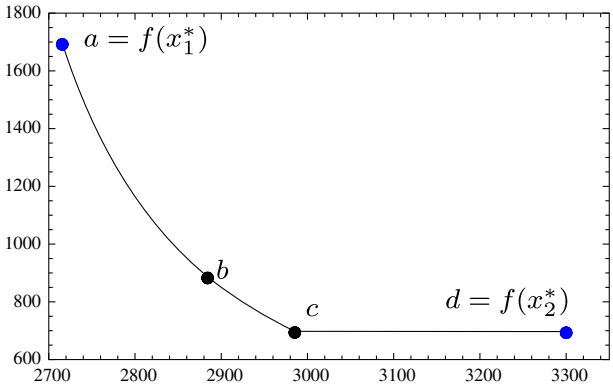

Fig. 3 Captured Pareto-optimal curve in the objective space

Table 1 Change of $\mathcal{A}$: + means activated, − means disactivated

Constraint	$a \to a$	$a \to b$	$b \to b$	$b \to c$	$c \to c$	$c \to d$	$d \to d$
g_8	−	−	+	+	+	+	+
$\underline{g}_{x_4}$	+	+	+	−	−	−	−
$\underline{g}_{x_6}$	+	−	−	−	−	−	−
$\overline{g}_{x_6}$	−	−	−	−	+	+	+
$\underline{g}_{x_3}$	+	+	+	+	+	−	−
g_{10}	−	−	−	−	−	−	+

reaching b, g_8 activates. Again, 7 constraints are active such that a path $b \to b$ is followed in the multiplier space until the detection of the disactivation of $\underline{g}_{x_4}$. The path $b \to c$ has 6 active constraints, and reaches c by activating the constraint $\overline{g}_{x_6}$. ParCont leaves c by disactivating $\underline{g}_{x_3}$. It can hence further move on the path from $c \to d$. At d, g_{10} activates and the set of active constraints form a square system of equations: a path in the multiplier space is followed. The process stops at d by detecting negative objective multipliers ($\lambda < 0$).

4 Conclusion

We have presented in this paper an overview of continuation techniques for NLBOO problems: local techniques that follow curves of (locally) Pareto-optimal solutions. Techniques based on the framework in [22], i.e. applying a continuation process on the system of first order optimality conditions without using any explicit parameter, have a better behavior than other approaches like methods based on the local solving of scalarized problems: although all suffer from loss of constraint qualification, [22] it is not subject to failure at turning points. However, such techniques proposed in the literature generally do not handle inequality constraints (changes of constraint activity yielding singularities of the system of first order conditions).

To overcome this limitation, we have introduced a certified continuation method for NLBOO, based on interval analysis, that handles inequality constraints through an active set management process. It certifies changes of constraints activity provided that these changes

are stable, i.e. they occur one at a time. Applied to a representative constrained problem, the approach shows its ability to track the Pareto-optimal curves with guarantee of feasibility and local optimality. Such certificates of feasibility are helpful in global solvers, e.g. population based algorithms or branch and bound, as they make it possible to accurately and rigorously construct bounds. The additional certificate of connectivity also provides some insights on the topology of the Pareto frontier. The process still has some limitations: the technique cannot track singularities other than constraint activations and it does not scale well to high-dimensional problems due to the cost of the certificates. This cost however seems reasonable for a usage within a global optimization method.

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